APPLICATIONS OF THE DEBYE SCATTERING EQUATION TO A CRYSTALLINE POWDER

A Thesis

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by

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CONTENTS

INTRODUCTION

The Debye Scattering Equation is used to calculate X-ray diffraction patterns of extremely small crystallites composed of a few tens to a few hundred unit cells. I have used the computer to perform the immense number of calculations involved and to plot the results. By varying crystallite dimensions, i.e. the shape of the crystallite, calculated peak intensities for certain powder lines depart from expected relative strengths. A shift of KA values for some peaks can also be observed. An attempt to correlate peak intensity with $1/d_{hkl}$ values ends with contradictory results.

SCATTERING OF X-RAYS - AN INTRODUCTION TO THE DEBYE EQUATION (AFTER AZÁROFF, pp.87,88,161-174)

Consider an unpolarized monochromatic X-ray beam encountering an electron at point O, as shown in Fig. 1. The average magnitude of the resultant electric field of the transverse wave at some point P (in the yz plane) is

$$\overline{\mathcal{E}_p^2} = \frac{\overline{\mathcal{E}_o^2}\, e^4}{r^2 m^2 c^4}\left(\frac{1+\cos^2\phi}{2}\right) \qquad (1\text{-}1)$$

where $\mathcal{E}$ = electric vector

e = charge of an electron

m = mass of an electron

c = velocity of light

r = distance from point O to point P

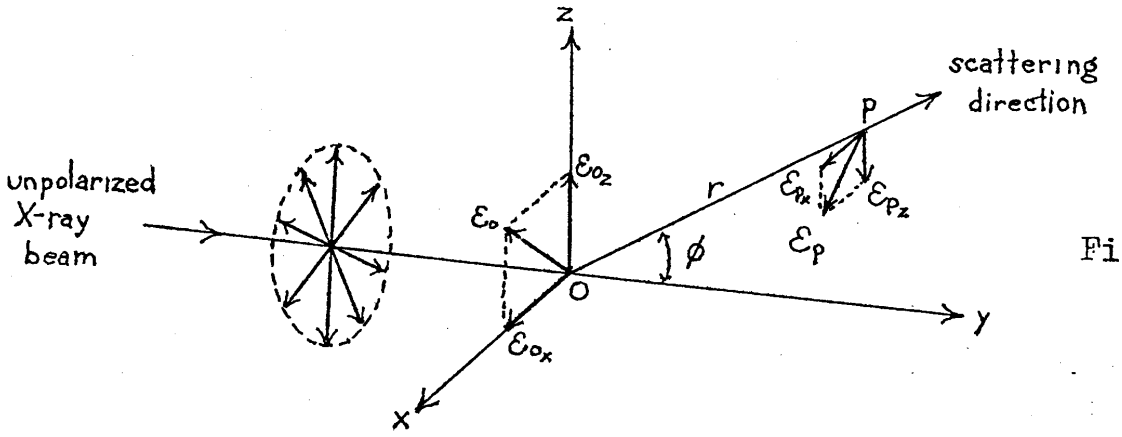


Figure 1.

The intensity of the beam $I=(c/4\pi)\mathcal{E}^2$ measures the energy crossing unit area per unit time. Multiplying (1-1) by $c/4\pi$ will give Thomson's equation:

$$I_e = I_o \frac{e^4}{r^2 m^2 c^4} \left(\frac{1+\cos^2 \phi}{2} \right) \qquad (1\text{-}2)$$

where I is the intensity of coherent scattering by one electron.

The ratio of the amplitude of the wave scattered by an atom and the amplitude of the wave scattered by an electron is called the atomic scattering factor, $f=\frac{Ea}{E_e}$ or $Ea=fE_e$. (1-3)
Squaring equation (1-3) and multipying both sides by $c/4\pi$ results with $Ia=f^2 I_e$, where Ia is the intensity of coherent scattering by an atom. Equation (1-4) expresses this intensity in electron units (eu).

$$Ieu = \frac{Ia}{I_e} = f^2 \qquad (1\text{-}4)$$

Let $\overline{r}_{mn}$ be the interatomic vector (i.e. the difference vector between the radius vectors of atoms m and n compared to

the origin atom), So the unit vector in the incident ray direction, and S the unit vector of the diffracted ray. (see Fig. 2.) The phase difference between the X-rays scattered by the atom m a distance Rm from the origin atom can be expressed by $e^{(2\pi i/\lambda)(\bar{S}-\bar{S}o)\cdot\bar{R}m}$, where e is the exponential function and i is the square root of -1. The total intensity scattered by all the atoms relative to the origin atom is the sum of the intensity scattered by each atom. The atoms, drawn as circles in Fig. 2, are considered to be in a gas. Each atom in the gas could have been the origin. This leads to the double summation

$$Ieu = \sum_m \sum_n f_m f_n e^{(2\pi i/\lambda)(\bar{S}-\bar{S}o)\cdot\bar{r}_{mn}} \qquad (1\text{-}5)$$

or, alternately

$$Ieu = \sum_m \sum_n f_m f_n e^{iKr_{mn}\cos\phi} \qquad (1\text{-}6)$$

where the dot product has been resolved, $K=\frac{4\pi\sin\Theta}{\lambda}$, and ϕ is the angle between $(\bar{S}-\bar{S}o)$ and $\bar{r}_{mn}$.

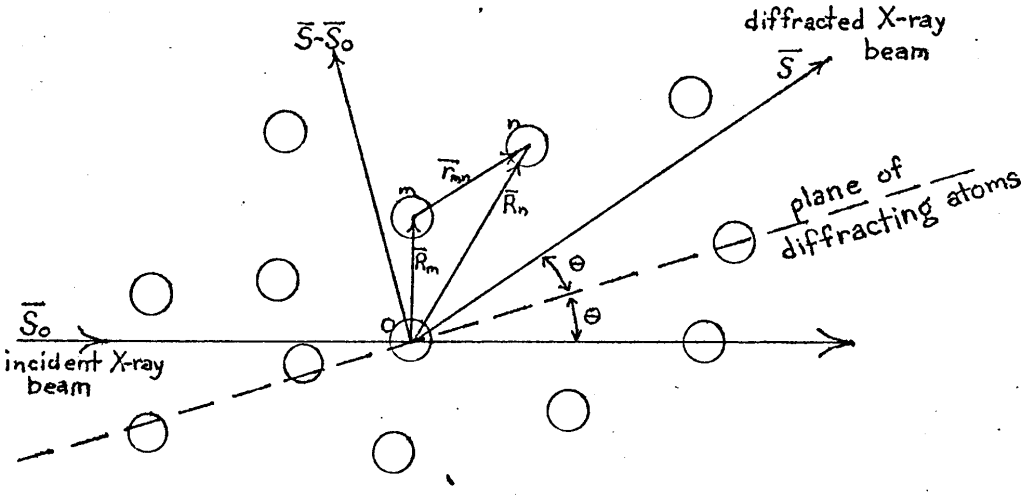


Figure 2.

Equation (1-6) is an accurate expression for the intensity at one instant in time. Averaging (1-6) over time (Azároff,p.174) gives

$$\overline{Ieu} = \sum_m \sum_n f_m f_n \frac{\sin Kr_{mn}}{Kr_{mn}} \qquad (1\text{-}7)$$

Equation (1-7) is called the Debye scattering equation, which is an expression for the time averaged unmodified intensity in electron units from an array of atoms which takes all orientations in space. This equation involves only the magnitudes of the distances, r_{mn}, of each atom from every other atom. The Debye scattering equation can be applied to any form of matter in which there is a random orientation. This includes gasses, liquids, amorphous solids and crystalline powders (Warren,p.116). Application to powder patterns can be obtained by considering each crystallite as a molecule. The unmodified intensity per crystal is given by

$$Ieu/Nf^2 = \sum_m \sum_n \frac{\sin (KAr_{mn})}{KAr_{mn}} \qquad (1\text{-}8)$$

where A is the cell edge in the Isometric system and N equals the number of crystals in the sample. The cell edge is equal to one for my study. If only one type of atom is considered then $f_m f_n = f^2$. If the like r_{mn} terms of the expansion are collected as r_i, Fr_i is the number of times this distance occurs in a given crystallite, and Q is the number of different unique distances, then

$$Ieu/Nf^2 = \sum_{i=1}^{Q} Fr_i \sin (KAr_i)/(KAr_i) \qquad (1\text{-}9)$$

The utility of this latter form of equation (1-8) is realized when the number of calculations involved in the two forms is compared with computer time. However, treatment of crystallites containing more than a thousand atoms demands excessive CPU time. See Appendix E.

THE COMPUTER PROGRAM

This program can be divided into three parts.

1. Generation and storage of the atomic coordinates,
2. Calculation of the interatomic distances and collection of the unique distances and the number of times each distance occurs,
3. Computing the Debye scattering equation.

Generation and Storage of Atomic Coordinates

Several items must be decided before calculation of the coordinates can begin, the first of which is the lattice type. Only the Isometric system is considered in this study, so there is a choice of three Bravais lattice types. The primitive isometric, which I have designated PI, has eight atoms in the unit cell. The body-centered cubic (BCC) has nine atoms in the unit cell. The face-centered cubic (FCC) has fourteen atoms in the unit cell. The number of lattice points per PI unit cell, BCC unit cell and FCC unit cell is one, two, and four respectively. The position of any lattice point in a cell may be given in terms of its coordinates. For each of these lattice types the origin was chosen as a corner atom. The body-centering translations, 000 and ½½½, and the face-centering translations, 000, 0½½, ½0½, ½½0, give the coordinates of the lattice points which

can be used to construct the respective crystal. Addition of a set of integral coordinates (e.g. 100 or 121) will give the coordinates of equivalent points in different unit cells. These lattice points represent centers of atoms composing the crystals in my study. The points choosen to be acted on by integral coordinates in the three lattice types considered are:

PI 000

BCC 000, ½½½

FCC 000, 0½½, ½0½, ½½0

These coordinates are supplied on data cards located after the //GO.DATA DD * card. The number of lattice points in a unit cell is designated by the constant AUN. The crystallite is "built" by addition of integral coordinates in the x-, y-, and z-directions. The generated atomic coordinates are stored in arrays to be used in the next part of the program.

Calculating the Unique Interatomic Distances and Their Frequencies

The interatomic distances are calculated by computing the distance between every atom in the crystallite to every other atom including itself. These values are not stored since they are not needed after they are calculated. Each distance is tested for uniqueness after it is calculated. An array labelled UNQDIS stores the values of unique distances. Another array, FRQDIS, records the number of times that a unique distance is repeated. The size of array UNQDIS equals the quantity Q in equation (1-9). A particular element in array UNQDIS represents r in the same equation. Fr in equation (1-9) is represented by an element

in array FRQDIS.

The number of unique distances may be only six, as is the case for a 1 X 1 X 1 FCC crystallite, or as many as 342 for the 1 X 4 X 18 FCC crystallite. A value of 500 is used in the program for the size of arrays UNQDIS and FRQDIS to avoid changing dimensions with a change of cell size. It is this part of the program that uses the most CPU time, so any time limitations must be considered carefully (see Appendix E). Shown below are formulas to calculate the total number of atoms in a "smooth surface" isometric crystal of any shape or size for each of the lattice types. NX is the number of unit cell repetitions in the x-axis direction, and similarly for NY and NZ in the y- and z-axis directions respectively.

FCC
$$\frac{(NX+1)(NY+1)(NZ+1) + (NX)(NY)(NZ+1) + (NX)(NY+1)(NZ) + (NX+1)(NY)(NZ)}{\text{total number of atoms}}$$

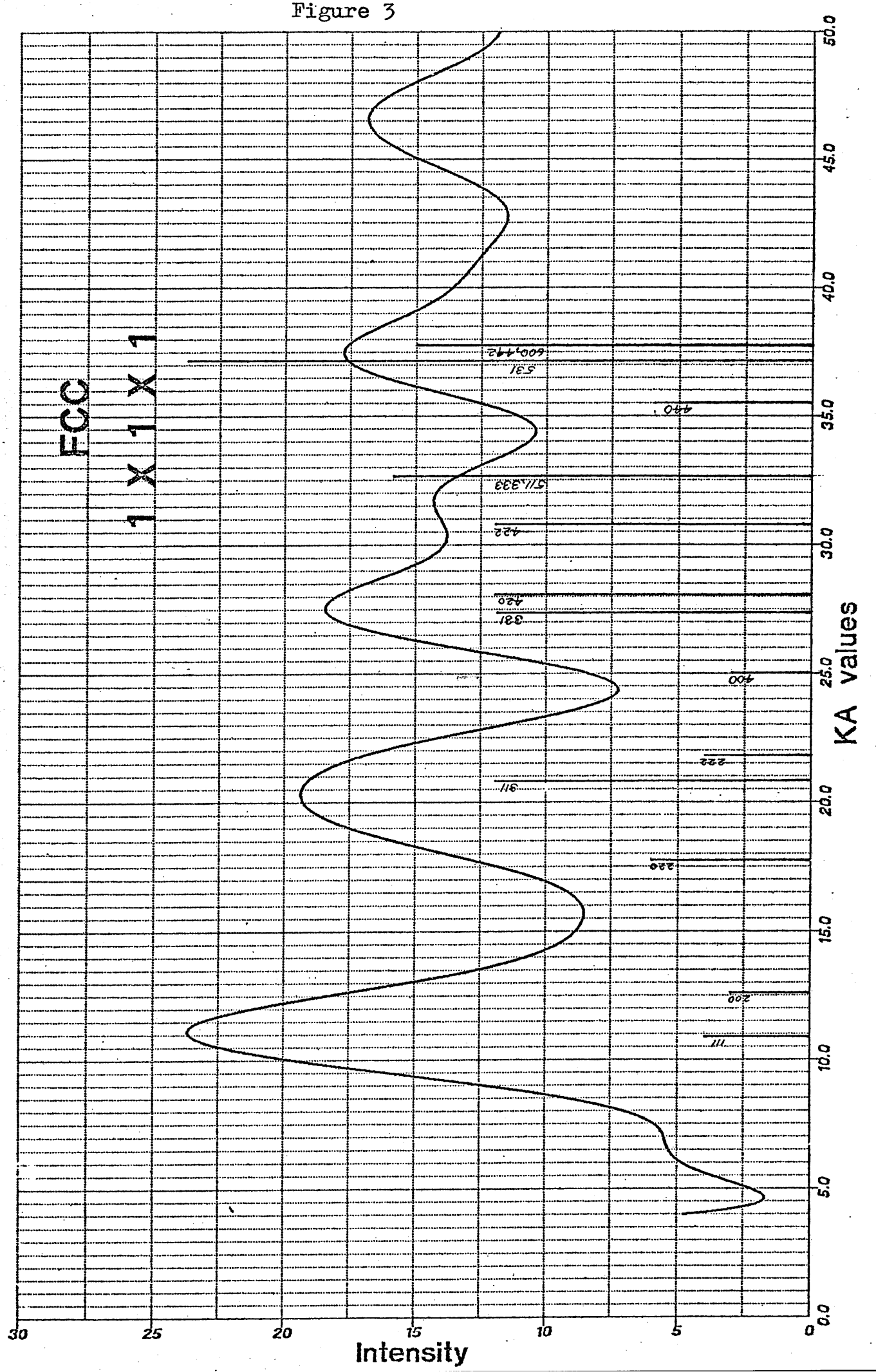
BCC
$$\frac{(NX+1)(NY+1)(NZ+1) + (NX)(NY)(NZ)}{\text{total number of atoms}}$$

PI
$$(NX+1)(NY+1)(NZ+1) = \text{total number of atoms}$$

Computing the Debye Scattering Equation

In order to reduce the number of calculations it is preferrable to use the Debye scattering equation as it appears in equation (1-9). This same equation was used by Warren. My plot of the intensity distribution pattern of a 1 X 1 X 1 FCC crystallite appears in Figure 3. The positions of the first

Figure 3


FCC
1 X 1 X 1
KA values
Intensity
0.0
5.0
10.0
15.0
20.0
25.0
30.0
35.0
40.0
45.0
50.0
0
5
10
15
20
25
30
111
200
220
311
222
400
331
420
422
511/333
440
531
600,442

thirteen FCC powder lines are indicated. The correlation is very close to the plots shown in Warren (p.119) and Hofmann (p.23).

KA values are calculated at 0.1 increments to increase the accuracy of locating peaks. A tally of peaks is kept by comparing each intensity to those at the previous and subsequent KA values. This part of the program is very similar to that in Hofmann (1976) which he wrote for a similar study. His system worked well so I made only minor modifications. I concentrated on developing the first two parts of this program.

The data may be printed out by either lineprinter or card punch. To use the plotting routines that I have formulated (Appendix A), KA and Intensity values are punched on cards for use as data entries. Storing these values on cards avoids having to repeat the calculations for use in further operations (plotting) or for comparison with other data.

DISCUSSION OF RESULTS

Four general crystallite shapes were chosen for study. They are listed in Table 1. Plots of the intensity distribution patterns for these five crystallites are shown in Figures 4 through 8. The positions of the first twenty-one FCC powder lines are indicated. Multiplicity factors are used to compare relative intensities of the powder lines for a crystal of very large size. Shown in Appendix D are some hkl indices corresponding to various KA values for an infinite crystal for comparison

Shape	Dimensions	Number of atoms	Number of different unique distances
Equant	5x5x5	666	98
Lathlike	1x4x18	500	342
Lathlike	2x2x20	513	277
Tabular	1x8x8	434	156
Rodlike	1x1x25	230	150

Table 1. Comparison of crystallites

with the peaks on my patterns of small crystallites. The equation $KA = 2\pi(h^2+k^2+l^2)$ was used to relate KA and hkl. See Appendix C for derivation of this relationship.

It is important to notice that although the Debye scattering equation does not make use of the structure factor directly, only the peaks that would be expected to appear for a chosen lattice type do appear in the plots. Plots of a 6x6x6 BCC crystallite and a 7x7x7 PI crystallite are shown in Figures 9 and 10 for comparison with the 5x5x5 FCC plot. The plots are in terms of Ieu/Nf^2 and the general variable KA.

A decline in intensity with increasing KA is apparent in every pattern. The reason for this is not obvious and requires closer study of the role of the Debye scattering equation (1-7). Equation (1-7) defines the intensity of scattering by a very small crystallite (less than 10^{-4} cm.) as a function of the scattering direction expressed in terms of the direction of incidence of the X-ray beam (proportional to K) and the structure of the crystal which is related to r . Maximum values occur when

Figure 4.

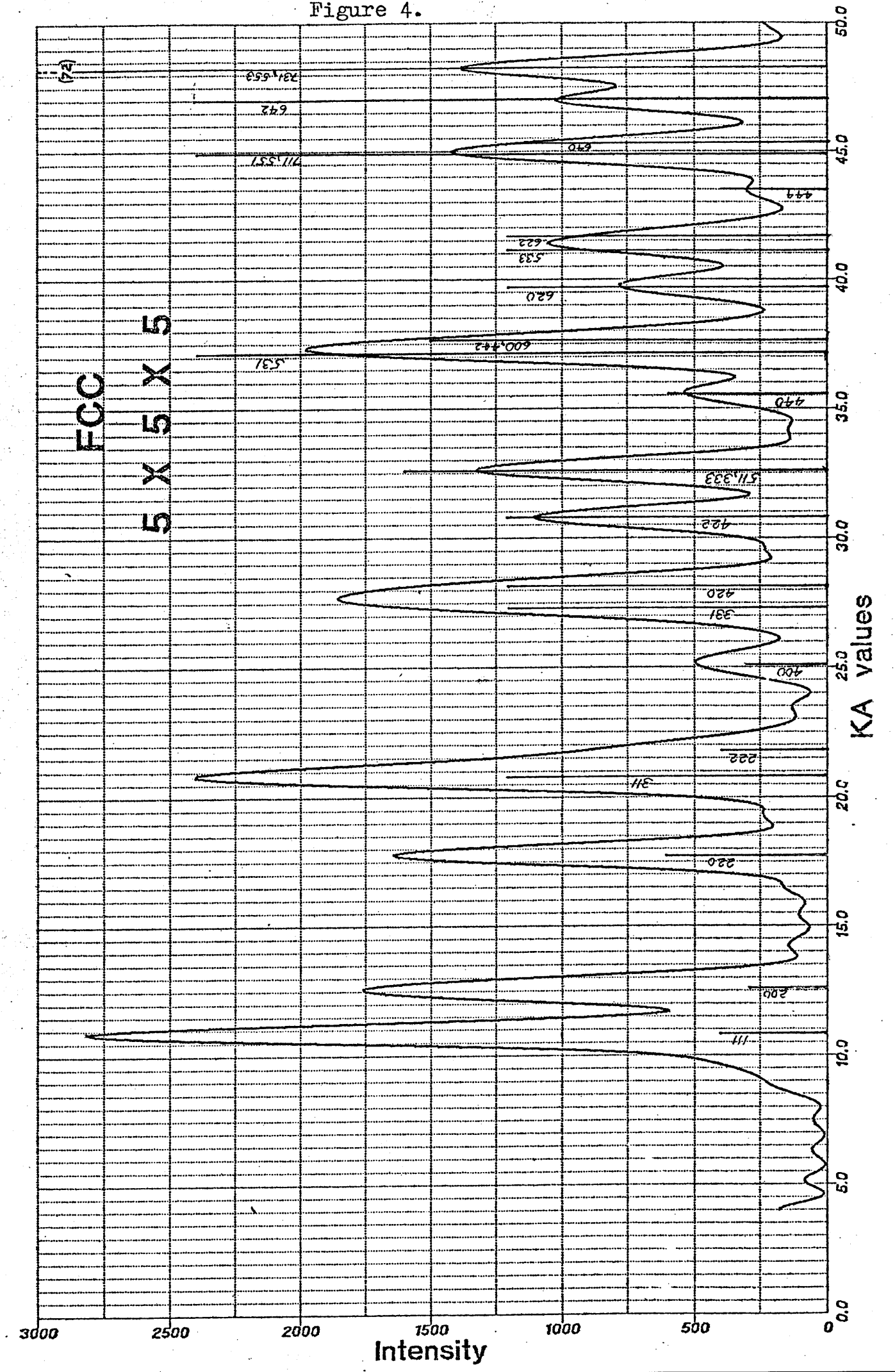

FCC
5 X 5 X 5
731,553
642
711,551
444
622
533
620
600,442
531
440
511,333
422
420
331
400
222
311
220
200
111
3000
2500
2000
1500
1000
500
0
Intensity
0.0
5.0
10.0
15.0
20.0
25.0
30.0
35.0
40.0
45.0
50.0
KA values

Figure 5

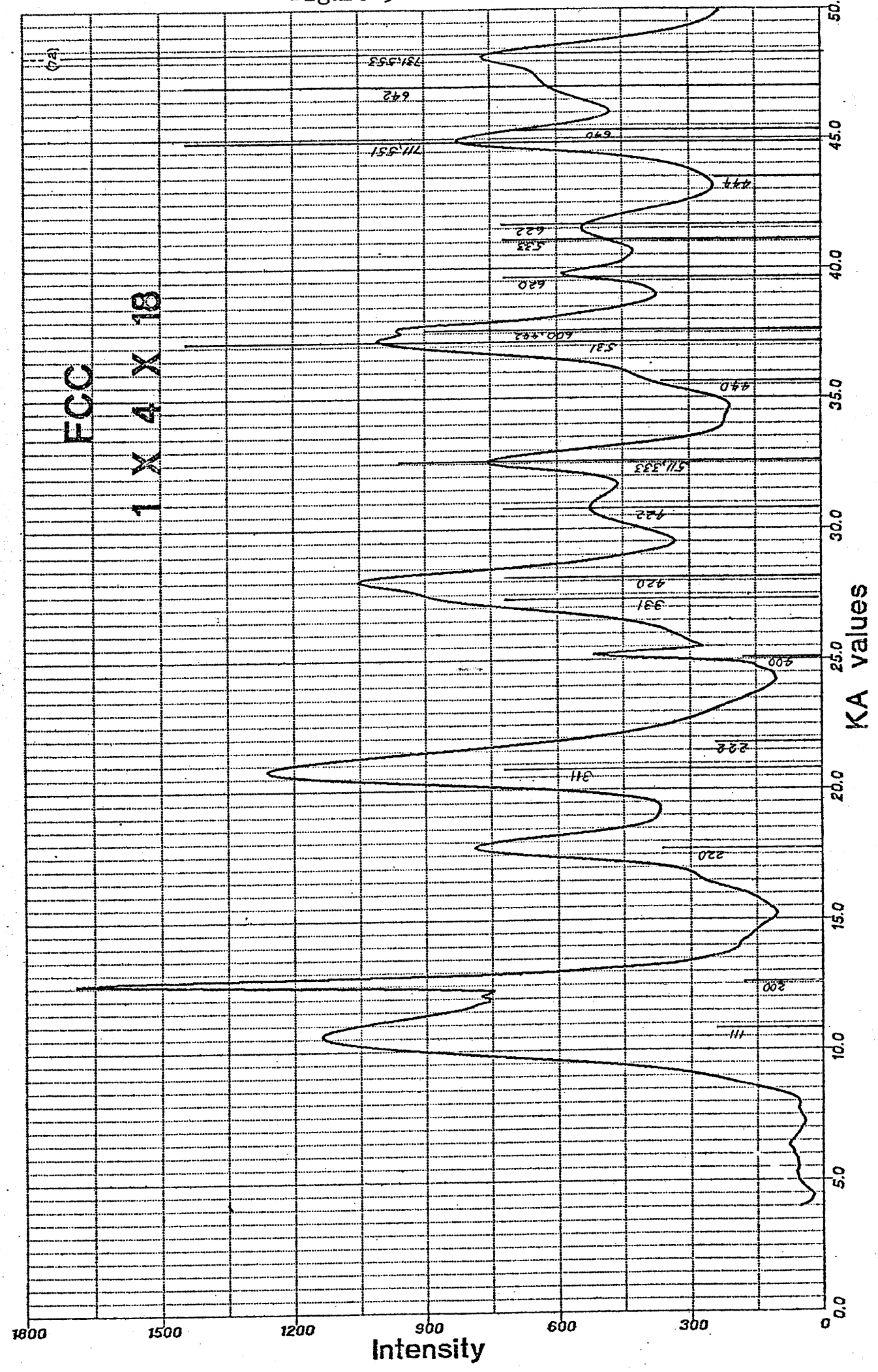

FCC
1 X 4 X 18
Cu Kα
731,553
642
620
711,551
444
622
533
620
600,442
531
440
511,333
422
420
331
400
222
311
220
200
111
50.0
45.0
40.0
35.0
30.0
25.0
20.0
15.0
10.0
5.0
0.0
KA values
1800
1500
1200
900
600
300
0
Intensity

Figure 6.

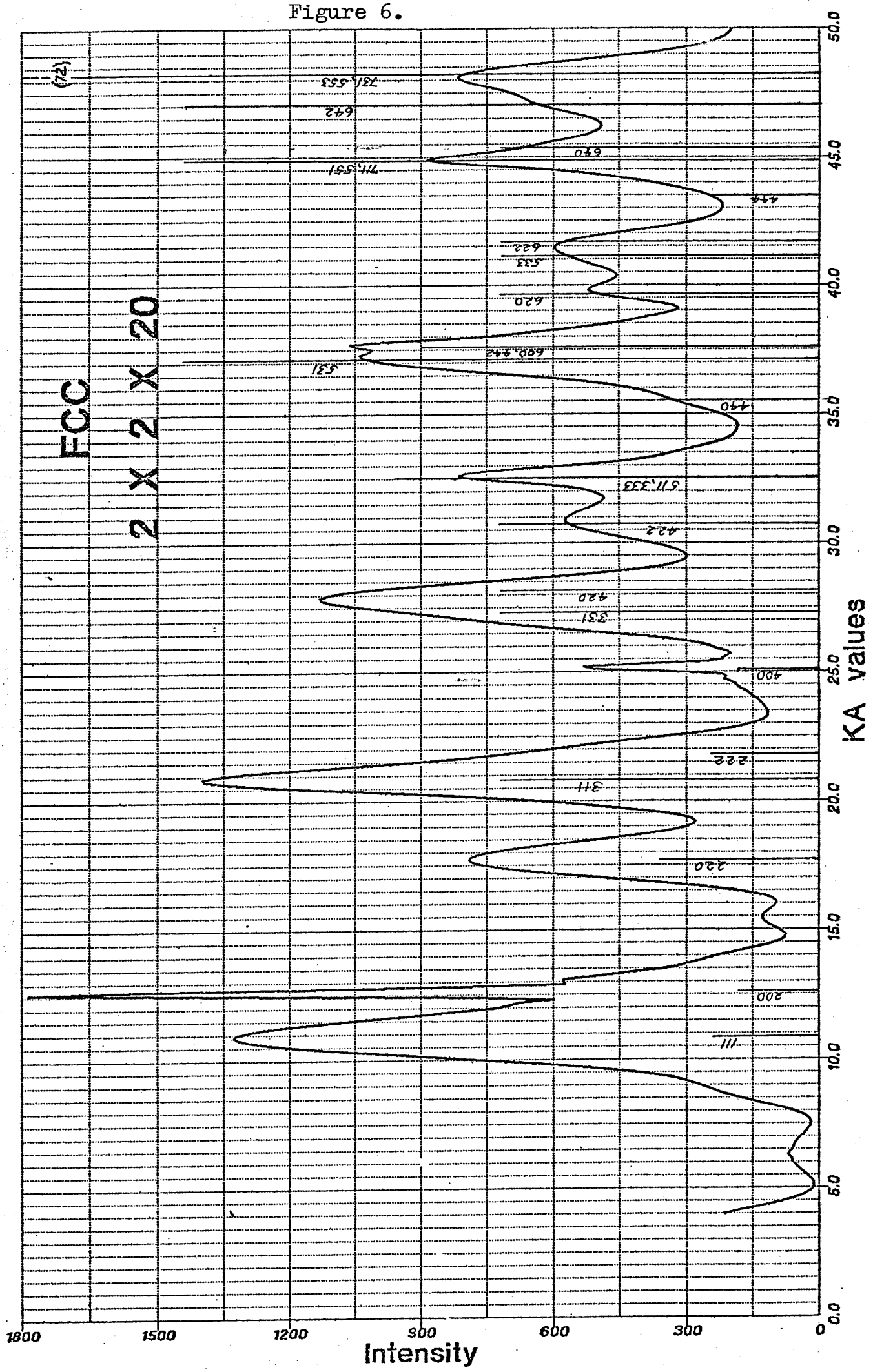

FCC
2 X 2 X 20
(72)
731, 553
642
640
711, 551
444
622
533
620
600, 442
531
440
511, 333
422
420
331
400
222
311
220
200
111
50.0
45.0
40.0
35.0
30.0
25.0
20.0
15.0
10.0
5.0
0.0
KA values
1800
1500
1200
900
600
300
0
Intensity

Figure 7.

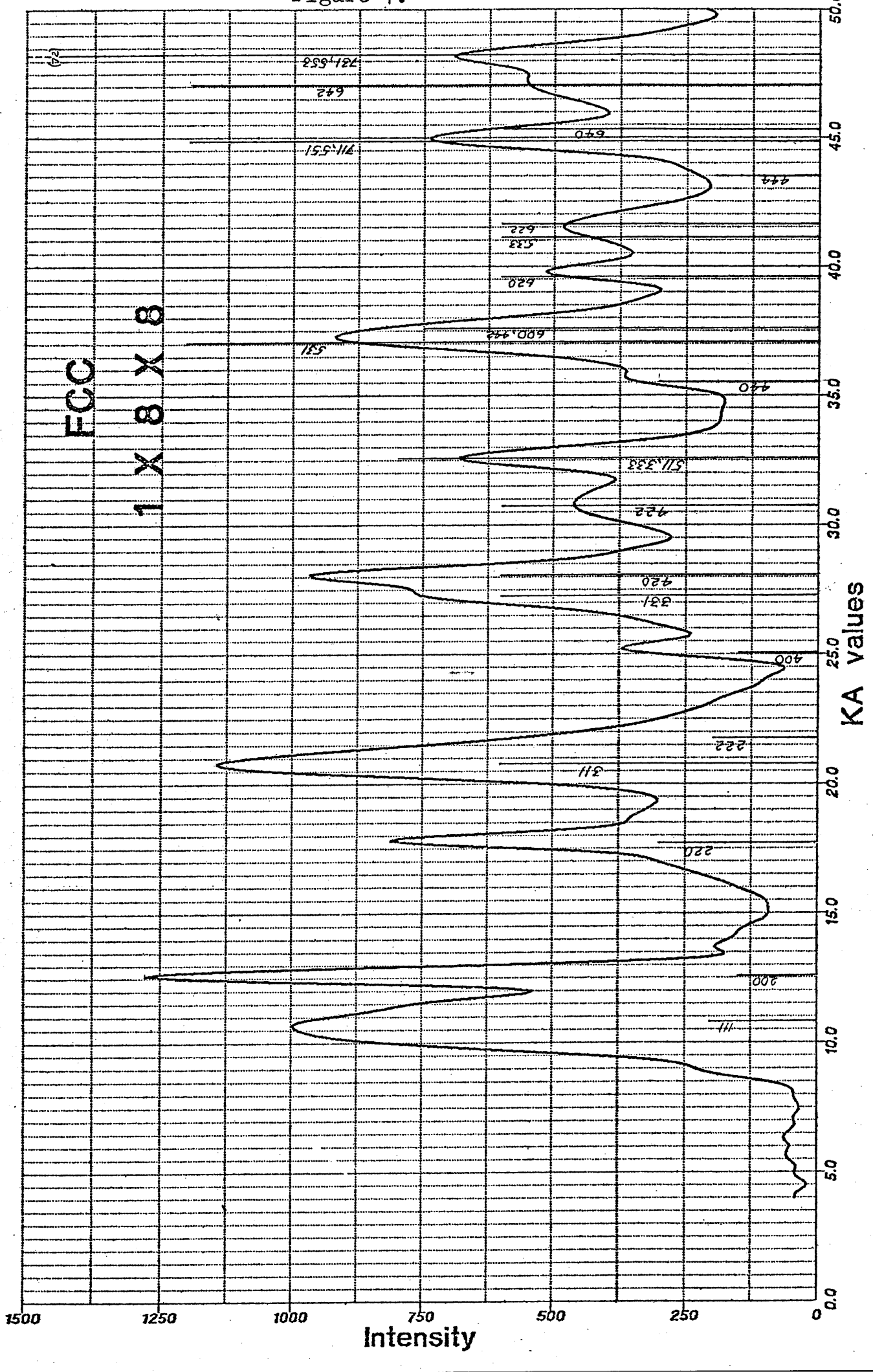

FCC
1 X 8 X 8
200
111
220
311
222
400
331
420
422
511,333
440
531
600,442
620
533
622
640
711,551
444
642
731,553
642
Intensity
1500
1250
1000
750
500
250
0
KA values
0.0
5.0
10.0
15.0
20.0
25.0
30.0
35.0
40.0
45.0
50.0

Figure 8.

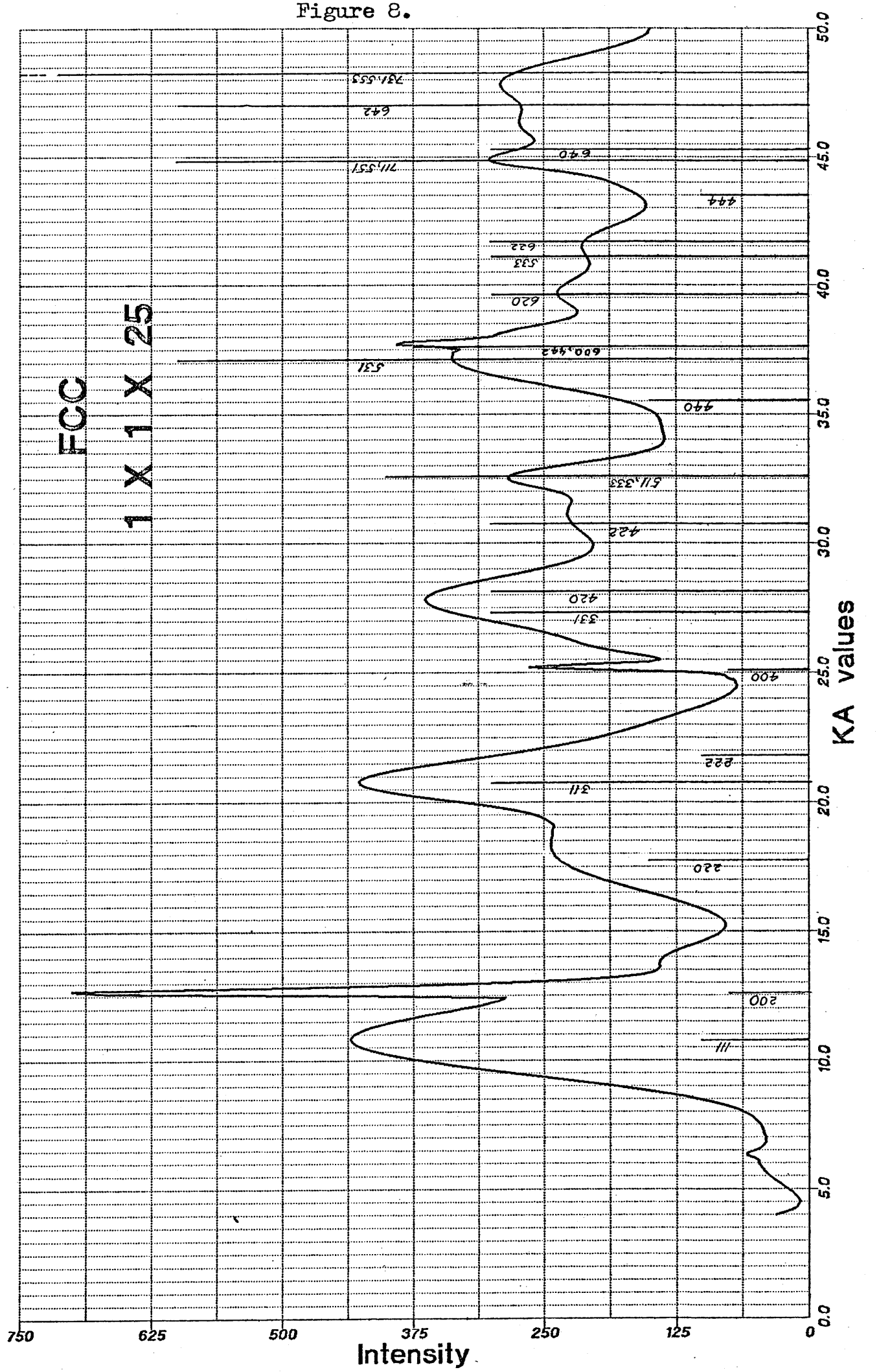

FCC
1 X 1 X 25
111
200
220
311
222
400
331
420
422
511,333
440
531
600,442
620
533
622
444
640
711,551
642
731,553
0.0
5.0
10.0
15.0
20.0
25.0
30.0
35.0
40.0
45.0
50.0
KA values
750
625
500
375
250
125
0
Intensity

Figure 9.

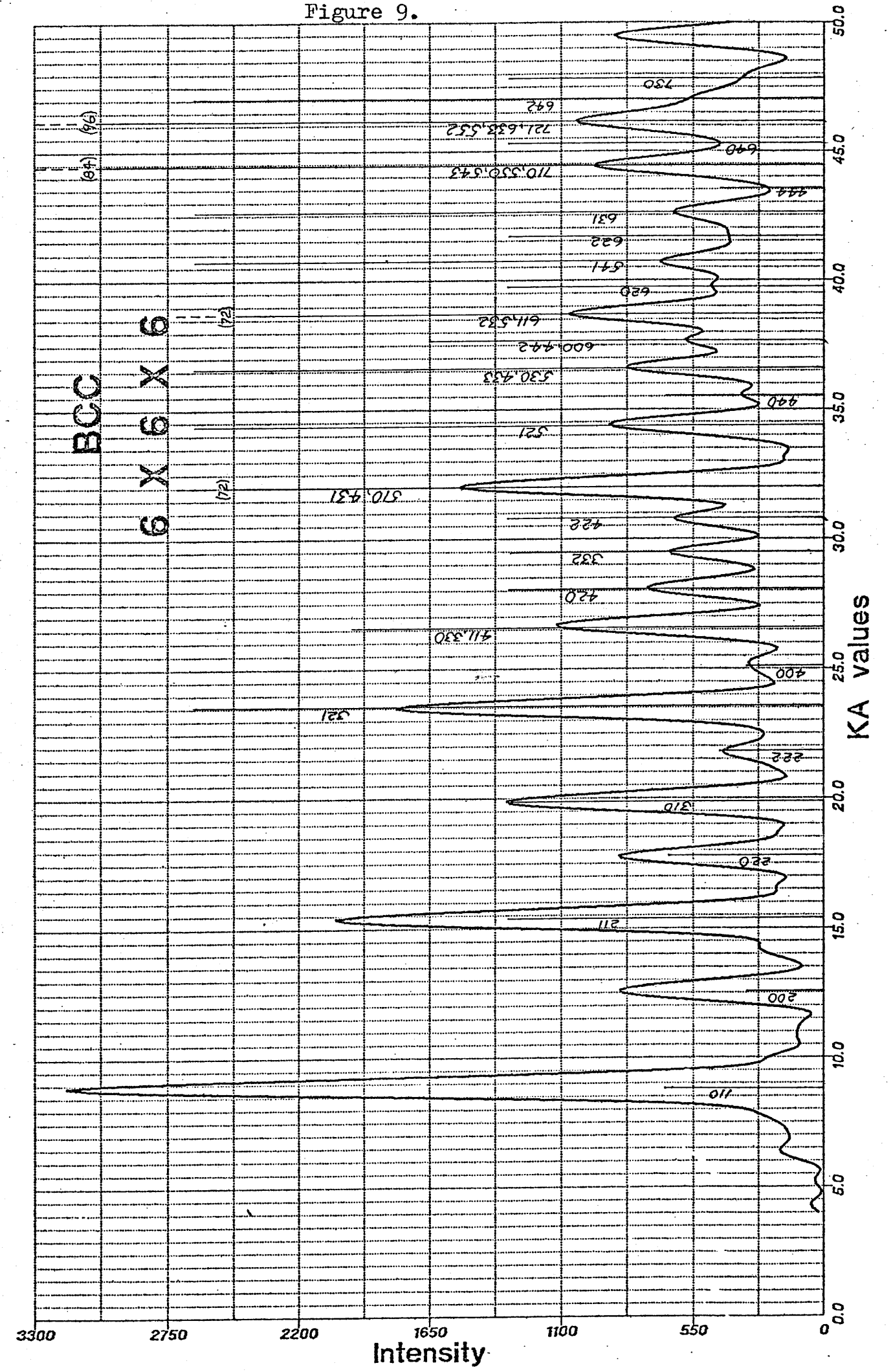
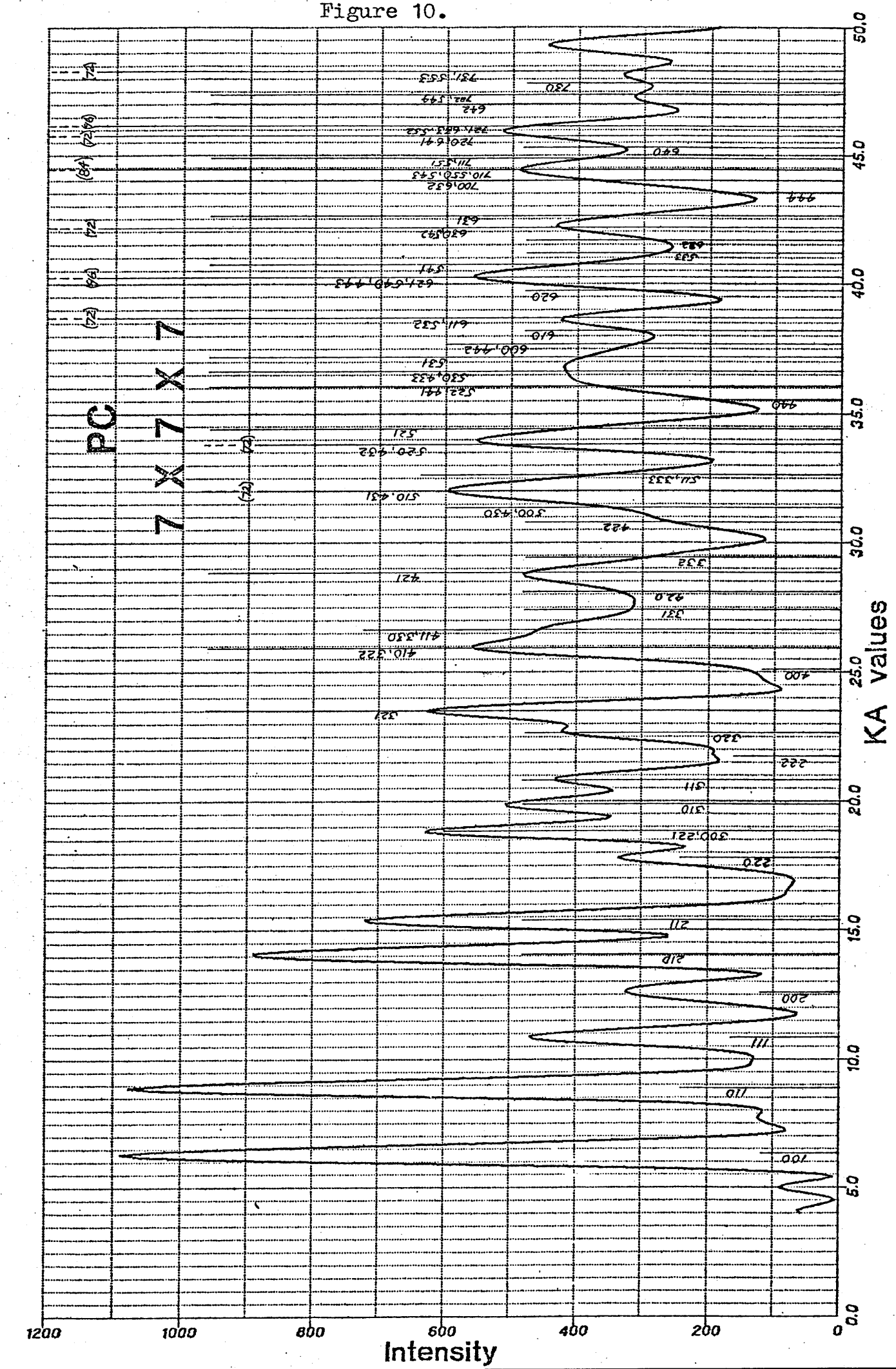

BCC
6 X 6 X 6
(72)
(72)
(84)
(96)
110
200
211
220
310
222
321
400
411,330
420
332
422
510,431
521
440
530,433
600,442
611,532
620
541
622
631
444
710,550,543
721,633,552
642
730
690
0.0
5.0
10.0
15.0
20.0
25.0
30.0
35.0
40.0
45.0
50.0
KA values
3300
2750
2200
1650
1100
550
0
Intensity

Figure 10.


PC 7 x 7 x 7
KA values
Intensity
0.0
5.0
10.0
15.0
20.0
25.0
30.0
35.0
40.0
45.0
50.0
0
200
400
600
800
1000
1200

the three Laue equations are satisfied, or when

$$K = \frac{4\pi \sin\Theta}{\lambda} = 2\pi\frac{\sqrt{h^2+k^2+l^2}}{A} \qquad (1\text{-}10)$$

where A is the unit cell length for an isometric crystal. (See Appendix C for derivation of (1-10).) When $h^2+k^2+l^2$ does not equal a whole number then an intensity less than the maximum results. The positions of the peaks (on the KA scale) are determined by the positions of the atoms in the the unit cell, represented in equation (1-9) by r_j, Fr_j, and Q. It would seem then that the resultant amplitude in the scattering direction from a small crystallite is the sum of the contributions from the unit cells with the phase differences taken into account. The phase difference from the contributions of the unit cells expressed as a time averaged value is

$$\overline{e^{(2\pi i/\lambda)(\bar{S}-\bar{S}o)\cdot\bar{R}m}} = \overline{e^{iKr_m\cos\phi}} = \frac{\sin Kr_{mn}}{Kr_{mn}}$$

This calculation is done by Azaroff (p.174). Using the Debye scattering equation in the form that it appears in equations (1-8) and (1-9) will result in a decrease in "intensity" with an increase in KA, because the "intensity" is the actual intensity divided by the square of the atomic scattering factor which is itself affected by the scattering direction. Also, as Kr_{mn} increases, the expression $\frac{\sin Kr_{mn}}{Kr_{mn}}$ deceases in value.

However, even though there is a decline in intensity with an increase in KA, when a small range of KA values is considered the ratio of the peak intensities of the reflections maintain their expected relations. Hofmann (1976) came to a similar

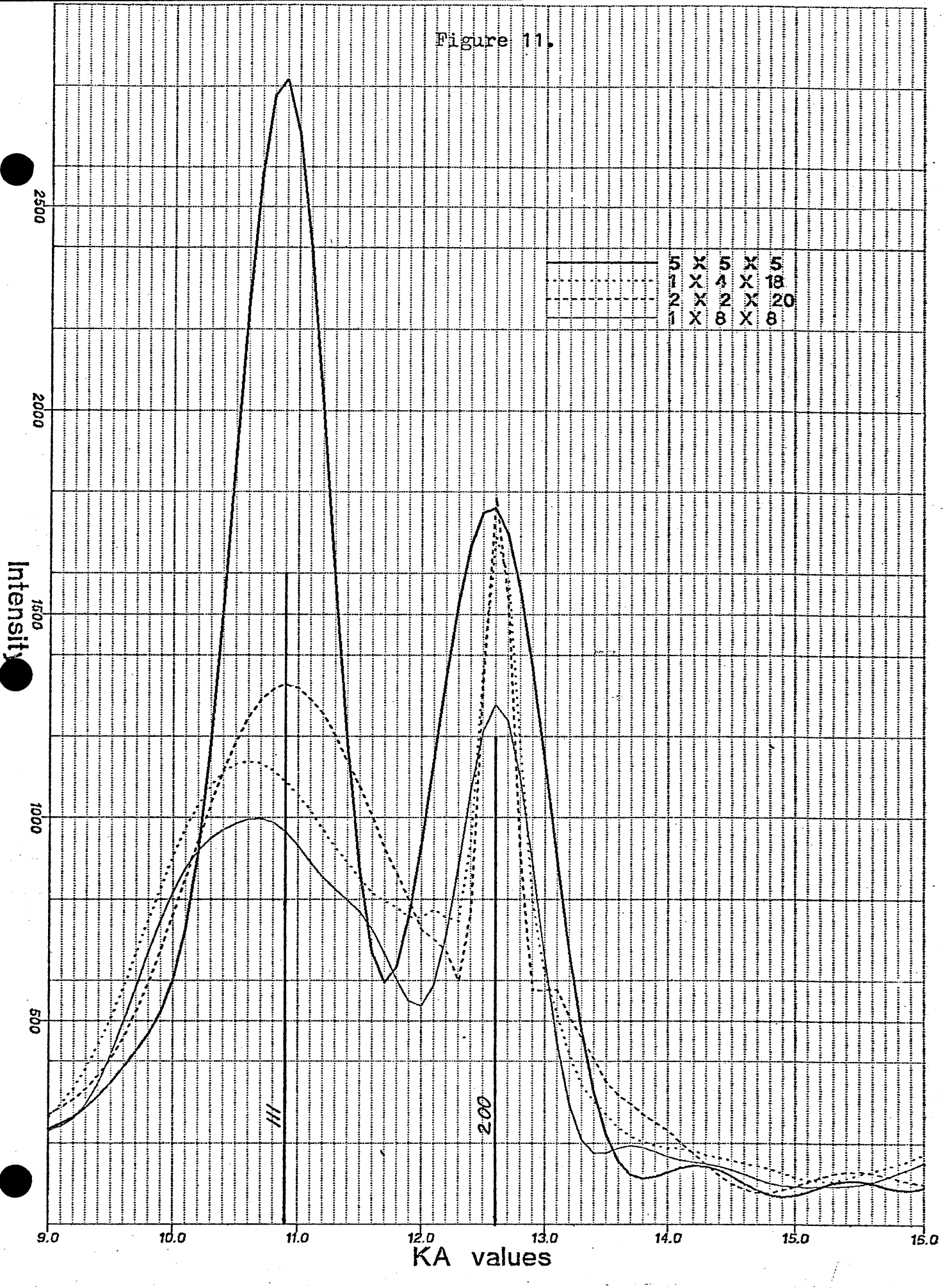
conclusion. For example, the 111 reflection (at KA 10.88) with a multiplicity (p) of 8 is a little higher than the 200 reflection (at 12.57) with p equal to 6. Also, the 220 reflection (at 17.77) with p 12 is a little less than the 311 reflection (at 20.84) with p 24. These two examples are from equant-shaped cells, but by varying the crystallite shape from equant different intensity ratios can be produced.

Figures 11,12 and 13 show four different crystallites compared over three limited KA ranges. Zachariasen (p.103) showed that the intensity associated with the diffracted wave decreases with decreasing crystal size. This is verified by these figures.

KA Values 9.0 to 16.0 (Fig. 11)

The intensity of the 111 reflection is greater than that for the 200 reflection in the 5x5x5 pattern. This is the predicted relation. But for every other crystallite shape the 111 peak intensity is less than the intensity of the 200 peak. This seems contradictory until the intensity for the reflection is integrated for the area under the curve. When this is done the total power of the 111 reflection is greater than that for the 200 reflection. This restores the normal relations of the peaks. Tables 2 and 3 were prepared to compare selected peak locations, r and Fr values for the crystallites. If $1/d_{hkl}$ values are represented by r values, then relative peak intensities may correspond to the presence or lack of r values and the number of times this value (as a distance) occurs in the crystallite. The

Figure 11.

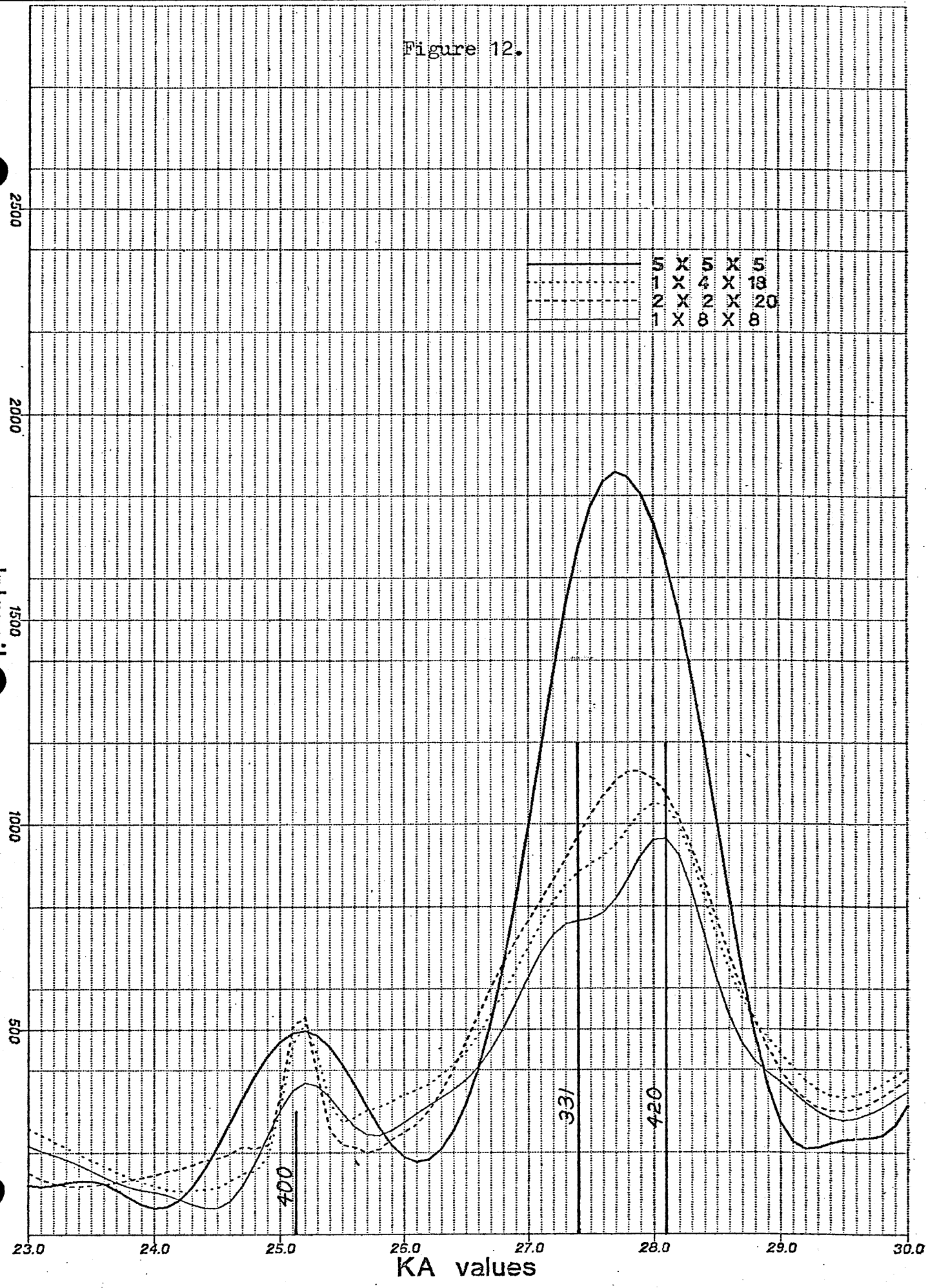

5 X 5 X 5
4 X 4 X 18
2 X 2 X 20
1 X 8 X 8
2500
2000
1500
1000
500
Intensity
111
002
9.0
10.0
11.0
12.0
13.0
14.0
15.0
16.0
KA values

r values corresponding to the $1/d_{hkl}$ values for the 111 and 200 reflections are present for all five crystallites but the ratios of the Fr values vary from crystallite to crystallite. These variations may account for the reversal of 111 and 200 peak intensities. The slight shift to lesser KA values of the 111 peak for the 1x4x18 and 1x8x8 patterns will be discussed later in this thesis.

KA Values 23.0 to 30.0 (Fig. 12)

Of greatest interest in comparing the patterns in this range is the beginning of resolution of the 331 and 420 reflections by the 1x8x8 (tabular) pattern and to a lesser extent by the 1x4x18 (lathlike) pattern. The resolution of the peaks must be caused by some particular arrangement of the unit cells. The 331 peak that is beginning to be resolved in the 1x4x18 and 1x8x8 plots does not appear as a peak in Table 2. The 420 peak does appear near the calculated value of 28.10 in the two patterns. In the other three crystallites these two peaks are not resolved but combined as one peak at an intermediate KA value of approximately 27.8. Table 3 shows that the r value which corresponds to the $1/d_{hkl}$ value is not present in the 2x2x20 and 1x1x25 crystallites. This may account for the lack of resolution in the patterns of these latter two crystallites. No explanation is offered for the presence of the r value of the 331 reflection in the 5x5x5 crystallite but lack of resolution of the 331 and 420 peaks. Additional investigation of larger crystallites may explain the resolution of these peaks

Figure 12.


5 X 5 X 5
1 X 4 X 13
2 X 2 X 20
1 X 8 X 8
2500
2000
1500
1000
500
Intensity
400
331
420
23.0
24.0
25.0
26.0
27.0
28.0
29.0
30.0
KA values

and those found in the next range of KA values discussed.

KA Values 35.0 to 42.0 (Fig. 13)

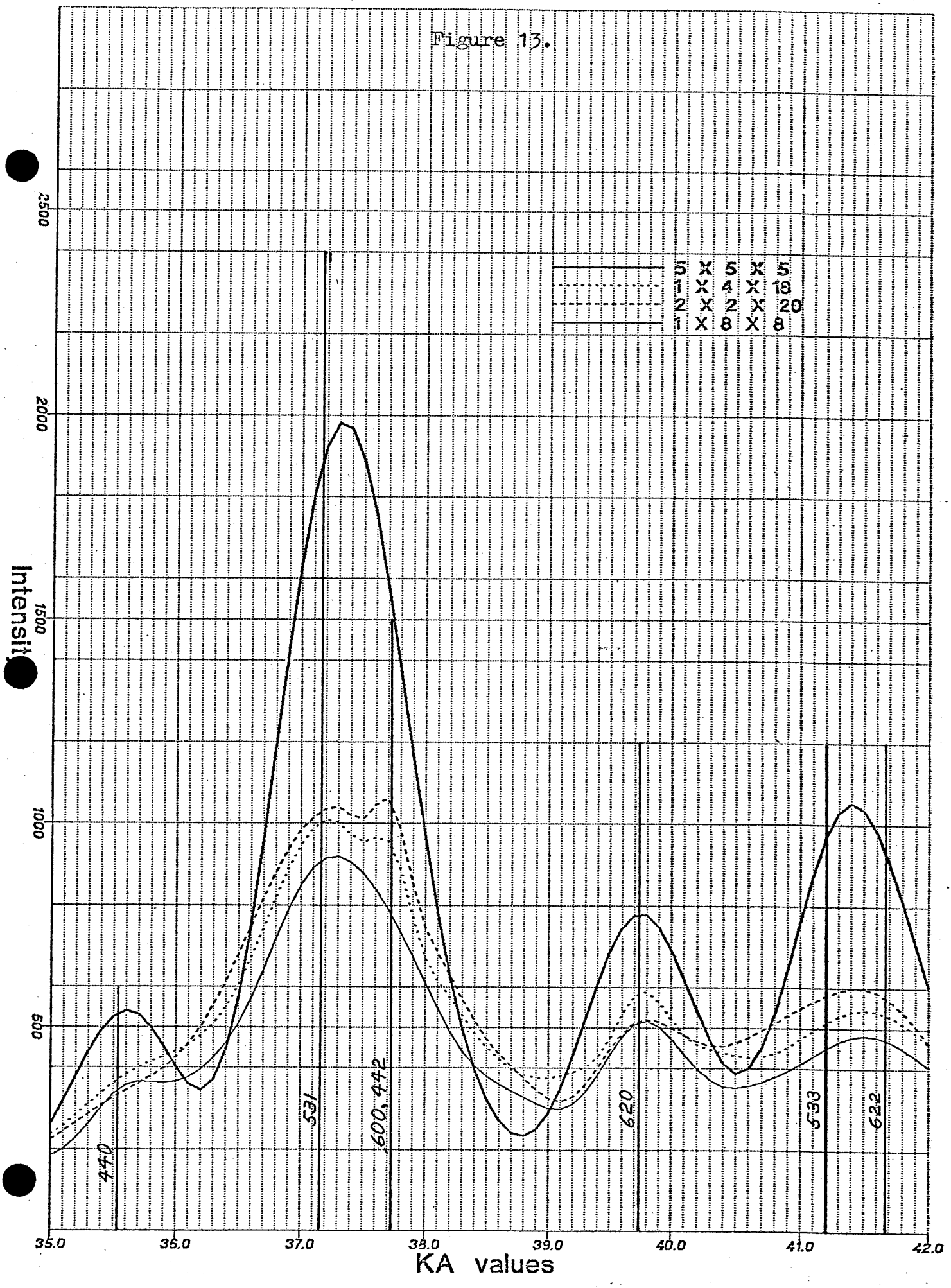
The 440 peak at KA 35.54 is missing entirely in the 2x2x20 pattern and the r value corresponding to $1/d_{440}$ does not appear in the 2x2x20 crystallite. The 440 peak starts to be resolved in the 1x4x18 pattern which may be accounted for by an r value equal to $1/d_{440}$ in the 1x4x18 crystallite. This same r value is present in the 5x5x5 and 1x8x8 crystallites and the peak is present also. This seems to indicate a positive correlation between presence of an r value and presence of the corresponding reflection.

Partial resolution of the 531 peak and the 600,442 peak is most apparent in the 2x2x20 pattern. The 531 peak is starting to appear but there is no r value equal to $1/d_{531}$ in the 2x2x20 crystallite. The 531 peak in the the 1x4x18 pattern is accompanied by the corresponding r value. But in contrast, the 5x5x5 and 1x8x8 crystallites also have the appropriate r value yet there is no resolution of the peaks. It seems then that there is no correlation between the presence of a certain $1/d_{hkl}$ value and the corresponding peak intensity in this KA range. Apparent correlations in other KA ranges may not then have any real significance.

Peak Shift

A comparison of Tables 2 and 3 shows that there is some correlation between peak shift and lack of the r value for that reflection. The largest shifts occur among the higher KA values.

Figure 13.


5 5 5
X X X
5 4 2
X X X
1 X 8 X 8
2500
2000
1500
1000
500
Intensit
35.0
36.0
37.0
38.0
39.0
40.0
41.0
42.0
KA values
440
531
400,442
620
633
622

The peak locations noted in Table 2 by an asterisk correspond to a lack of r values for those peaks in Table 3. A lack of an r value though does not mean there will be a peak shift. The shift of the 111 peak for the 1x4x18 and 1x8x8 patterns cannot be explained by presence or lack of the $1/d_{111}$ value. Additional investigation is warranted.

Conclusions

The patterns calculated using the Debye scattering equation show definite changes in the shape of the intensity distribution curves for various sizes and shapes of crystallites. These changes appear to be more the result of crystallite shape than of size. This observation may be useful in identifying the shapes of extremely small (less than 10^{-4}cm.) real crystallites. An explanation for the resolution or shift of certain peaks resulted in contradictory correlations. There was a positive correlation between peak resolution in the lower KA values and the presence of $1/d_{hkl}$ values for these peaks. For higher KA values there seemed to be no correlation at all. Additional investigation with larger FCC crystallites and with BCC and PI crystallites may resolve this conflict.

(hkl) Line	111	331	420	440	531	600,442	444	642	731,553
KA Value	10.88	27.39	28.10	35.54	37.17	37.70	43.53	47.02	48.26
FCC Crystallite									
5x5x5	10.9		27.7	35.6		37.3	43.5	47.0	48.3
1x4x18	10.6		28.0	—	37.2	37.6	—	—	48.2
2x2x20	10.9		27.9	—	37.3*	37.7	—	—	48.1*
1x8x8	10.7		28.1	35.7		37.3	—	47.2*	48.2
1x1x25	10.8		27.8	—	37.2*	37.7	—	46.3*	47.8*

Table 2. Selected Peak Locations.

(hkl) Line	111	331	420	440	531	600,442	444	642	731,553
$r = 1/d_{hkl}$	1.732	4.359	4.472	5.657	5.916	6.000	6.928	7.483	7.681
FCC Crystallite	F R E Q U E N C I E S								
5x5x5	2920	2712	2784	600	1104	768	112	—	72
1x4x18	984	376	1072	176	328	676	—	—	280
2x2x20	1408	—	664	—	—	726	—	—	—
1x8x8	904	488	1408	488	624	512	—	—	727
1x1x25	200	—	—	—	—	352	—	—	—

Table 3. Selected r and Fr values.

APPENDIX A

Herein are provided copies of the main program and the plot programs. The plotting programs are designed to be used with data entries punched on cards by the main program. The main program will produce output similar to that shown in Appendix B. The first plotting program produced Figures 3 through 10. The second plotting program produced Figures 11 through 13. FORTRAN IV coding was used throught with the additional consideration of the PPEP/EPS Subroutines for use of the Versatec plotter. The programs were run through the Ohio State University IBM 370 computer system. The Versatec plotter is located on the fifth floor of the Baker Systems Engineering Building, Neil Ave.

```
// REGION=300K,TIME=4
/*JOBPARM CARDS=100
//THESIS   EXEC PROC=SUPER,LIB='SYS1.FORTLIB',C=FORT,TIME.GO=(3,45)
//GO.SOURCE   DD *
C
C    F LATTICE
C  FCC    5 X 5 X 5
C
C  THIS PROGRAM WILL GENERATE AND STORE ATOMIC COORDINATES FOR THE GIVEN LATTICE
C    TYPE AND CELL SIZES.IT CALCULATES THE UNIQUE INTERATOMIC DISTANCES AND THEIR
C    FREQUENCIES.THEN CALCULATES THE DEBYE SCATTERING EQUATION.RESULTS ARE OUTPUT
C    BY LINE PRINTER AND/OR CARD PUNCH. X, Y, AND Z ARRAYS ARE THE TOTAL NUMBER
C    OF ATOMS IN THE CRYSTAL. 670 IS ADEQUATE FOR CELLS UP TO 5 X 5 X 5. XAL, YAL
C    , AND ZAL ARE THE AXIAL LENGTHS, EQUAL TO ONE HERE. AUN IS THE NUMBER OF
C    ATOMS IN THE UNIT CELL AND MUST BE CHANGED WITH A CHANGE OF LATTICE TYPE.
C    THE UNIT CELL ATOMIC COORDINATES ARE SUPPLIED ON DATA CARDS, WITH 5 SPACES
C    FOR EACH REAL COORDINATE. NX, NY, AND NZ ARE THE NUMBER OF REPITITIONS OF
C    THE UNIT CELL IN THE X, Y, AND Z AXIAL DIRECTIONS. TO CHANGE LATTICE TYPE
C    CHANGE AUN AND UNIT CELL COORDINATES. TO CHANGE CELL SIZES CHANGE NX, NY, NZ
C    PARAMETERS. THE SIZES OF UNQDIS AND FRQDIS ARRAYS ARE SUFFICIENT FOR THOSE
C    CRYSTAL SIZES TESTED
      REAL KAOFMX,INTMAX,INT1,KAI4631,INTI4631/463*0./,PEAK(75),R(75)
      DIMENSION XU(4),YU(4),ZU(4)
      INTEGER*2 AUN/4/
      DIMENSION X(670),Y(670),Z(670)
      REAL UNQDIS(500)/500*0./,FRQDIS(500)/500*0./
      DATA NX/5/,NY/5/,NZ/5/
      DATA XAL/1./,YAL/1./,ZAL/1./
      READ(5,3)(XU(I),YU(I),ZU(I),I=1,AUN)
    3 FORMAT(12F5.1)
      LX=NX+1
      LY=NY+1
      LZ=NZ+1
      N1=1
      DO 10 L=1,AUN
  110 DO 10 I=1,LX
      DO 10 J=1,LY
      DO 10 K=1,LZ
      X(N1)=XU(L)+((I-1)*XAL)
      Y(N1)=YU(L)+((J-1)*YAL)
      Z(N1)=ZU(L)+((K-1)*ZAL)
      IF(X(N1).GT.NX)GO TO 10
      IF(Y(N1).GT.NY)GO TO 10
      IF(Z(N1).GT.NZ)GO TO 10
      N1=N1+1
   10 CONTINUE
  111 N=N1-1
C
C COMPUTE STORE AND PRINT FREQ AND NO. OF UNIQUE INTERATOMIC DIS.
      NTOTAL=0
      DO 70 J=1,N
      DO 70 K=1,N
      DIST=SQRT((X(J)-X(K))**2+(Y(J)-Y(K))**2+(Z(J)-Z(K))**2)
      IF(J.EQ.1.AND.K.EQ.1) GO TO 1000
      IF(J.EQ.1.AND.K.EQ.2) GO TO 1001
      DO 71 L=1,NTOTAL
      IF(DIST.EQ.UNQDIS(L)) GO TO 1002
      IF(L.EQ.NTOTAL.AND.DIST.NE.UNQDIS(L)) GO TO 1003
   71 CONTINUE
 1000 UNQDIS(1)=DIST
      FRQDIS(1)=FRQDIS(1)+1.
      NTOTAL=NTOTAL+1



      GO TO 70
 1001 UNQDIS(2)=DIST
      FRQDIS(2)=FRQDIS(2)+1.
      NTOTAL=NTOTAL+1
      GO TO 70
 1002 FRQDIS(L)=FRQDIS(L)+1.
      GO TO 70
 1003 NTOTAL=NTOTAL+1
      UNQDIS(NTOTAL)=DIST
      FRQDIS(NTOTALT=FRQDIS(NTOTALT+1.
      GO TO 70
   70 CONTINUE
      KK=NTOTAL
C
C  COMPUTE THE DEBYE SCATTERING EQUATION
      INTMAX=0.0
      AMIN=100.0
      G=0.0
      INT1=0.0
      DO 80 I=1,KK
   80 G=G+FRQDIS(I)
      KI=1
      DO 81 I=1,461
      DO 81 J=1,KK
      IF(I.GT.3) GO TO 800
      IF(J.GT.1) GO TO 801
```

```
      GO TO 800
  801 CONTINUE
      IF(J.NE.KK) GO TO 800
      G1=SQRT(G)
  800 CONTINUE
      IF(UNQDIS(J).EQ.0.0) GO TO 802
      AI=I
      KA(I)=.1*AI+3.9
      F=KA(I)*UNQDIS(J)
      INT1=FRQDIS(J)*SIN(F)/F
      GO TO 803
  802 INT1=FRQDIS(J)
  803 INT(I)=INT(I)+INT1
      IF(J.LT.KK) GO TO 81
      IF(INT(I).LE.INTMAX) GO TO 804
      INTMAX=INT(I)
      KAOFMX=KA(I)
  804 IF(AMIN.LE.INT(I)) GO TO 805
      AMIN=INT(I)
      AKA=KA(I)
  805 CONTINUE
      IF(I.LT.5) GO TO 81
      LM2=I-1
      LM4=I-2
      IF(INT(I).LT.INT(LM2).AND.INT(LM2).GT.INT(LM4)) GO TO 806
      GO TO 81
  806 PEAK(K1)=INT(LM2)
      R(K1)=KA(LM2)
      K1=K1+1
      K1K=K1-1
   81 CONTINUE
C
C  PRINT OUT RESULTS
      WRITE(6,200)
      WRITE(6,201)
      WRITE (6,210)(I,X(I),Y(I),Z(I),I=1,N)



      WRITE(6,500)
      WRITE(6,501) (I,UNQDIS(I),FRQDIS(I),I=1,KK)
      WRITE (6,31) NX,NY,NZ
      WRITE(6,24)
      WRITE(6,25)(KA(I),INT(I),I=1,461)
      WRITE(7,300) (KA(I),INT(I),I=1,461)
      WRITE(6,26) INTMAX,KAOFMX
      DO 82 I=1,K1K
      WRITE(6,27) PEAK(I),R(I),I
   82 CONTINUE
  200 FORMAT('1',50X,'ATOMIC COORDINATES IN ANGSTROMS'//'0',' ')
  201 FORMAT('0',3(5X,'ATOM',5X,'X-AXIS',2X,'Y-AXIS',2X,'Z-AXIS',5X)//)
  210 FORMAT (3(5X,I4,2X,3F8.2,5X))
  500 FORMAT('0',50X,'INTERATOMIC DISTANCE    FREQUENCY'//)
  501 FORMAT(' ',53X,I4,5X,F8.3,3X,F7.1)
   24 FORMAT (//,6X,4(' KA        INTENSITY',6X)//)
   25 FORMAT (4(5X,F4.1,3X,F13.2))
   26 FORMAT('1',24X,'INTENSITY MAXIMUM OF ',F9.2,2X,' AT A KA VALUE OF
     1',F4.1///)
   27 FORMAT(10X,'THERE IS A PEAK OF INTENSITY OF ',F9.2,2X,' AT A KA VA
     1LUE OF ',F4.1,15X,I5/)
   31 FORMAT('1',50X,'FCC   ',I2,' X ',I2,' X ',I2)
  300 FORMAT(5(F5.1,F9.3))
C
      STOP
      END
/*
//GO.DATA    DD *
 0.0   0.0   0.0   0.0   0.5   0.5   0.5   0.0   0.5   0.5   0.5   0.0
/*
//
```

```
// REGION=192K
//THESIS   EXEC PLOTV
//GO.OBDECK DD DSN=SAA000.PLOTLIB.DISP=SHR
//GO.SOURCE  DD *
C  FCC       5 X 5 X 5
C
      DIMENSION H(20)
      REAL KA(463),INT(463)
      REAL INCRX/1./,INCRY/.333333/
      DATA NX/7/,NY/30/
C
      READ(5,300) (KA(I),INT(I),I=1,461)
  100 FORMAT(20A4)
  300 FORMAT(5(F5.1,F9.3))
C
      CALL PLOTS(0,0,C)
      CALL GRID(0.,0.,100.,1.,-60.,1.,4369)
      CALL GRID(0.,0.,10.,1.,12.,.5,13107)
C
C  DRAW X AXIS
      CALL HLINE(0.,10.,0.,65535)
      DO 40 I=1,10
      XTIC=I
   40 CALL VLINE(0.,-.065,XTIC,65535)
      READ(5,100) H
      CALL CCFONT(5.,-.34,.15,H,0.,-9,8,0.,1.,.01)
      DO 41 I=1,11
      FPNX=5.*(I-1)
      XCNTX=I-1
      YCNTX=-.15
   41 CALL NCFONT(XCNTX,YCNTX,.075,FPNX,0.,1,8,10.,1.,.01)
C  DRAW Y AXIS
      CALL VLINE(0.,6.,0.,65535)
      DO 42 I=1,6
      YTIC=I
   42 CALL HLINE(0.,-.065,YTIC,65535)
      READ (5,100) H
      CALL CCFONT(-.34,3.,.15,H,270.,-9,8,0.,1.,.01)
      DO 43 I=1,7
      FPNY=500.*(I-1)
      YCNTY=I-1
      XCNTY=-.15
   43 CALL NCFONT(XCNTY,YCNTY,.075,FPNY,270.,-1,8,10.,1.,.01)
C  PLOT INDIVIDUAL PATTERN
      CALL NEWPEN(3)
      CALL PLOT(KA(1)/5,INT(1)/500,3)
      DO 1 I=1,461
      CALL PLOT(KA(I)/5,INT(I)/500,2)
   1  CONTINUE
      READ(5,100) H
      CALL CCFONT(7.,5.,.2,H,0.,10,8,0.,1.,.01)
      READ(5,100) H
      CALL CCFONT(7.,5.5,.2,H,0.,3,8,0.,1.,.01)
      CALL PLOT(0.,0.,999)
C
      STOP
      END
/*
//GO.DATA    DD *
        REMOVE THIS CARD AND PUT DATA CARDS FOR CRYSTAL HERE
KA VALUES
INTENSITY



5 X 5 X 5
FCC
//GO.PLOTPARM  DD *
 &PLOT XMIN=-.5,XMAX=12.,YMIN=-.5,YMAX=10.06,MSGLVL=2  &END
/*
//PLOT.SYSVECTR DD SYSOUT=(A,,61),DEST=PLOT11
//
```

```
// REGION=192K
/*JOBPARM LINES=2000
//THESIS    EXEC PLOTV
//GO.OBDECK DD DSN=SAA000.PLOTLIB,DISP=SHR
//GO.SOURCE   DD *
C     5 X 5 X 5       1 X 4 X 18       2 X 2 X 20          1 X 8 X 8
      REAL KA1(463),INT1(463)
      REAL KA2(463),INT2(463)
      REAL KA3(463),INT3(463)
      REAL KA4(463),INT4(463)
      DIMENSION H(20)
C
      READ(5,300) (KA1(I),INT1(I),I=1,461)
      READ(5,300) (KA2(I),INT2(I),I=1,461)
      READ(5,300) (KA3(I),INT3(I),I=1,461)
      READ(5,300) (KA4(I),INT4(I),I=1,461)
  100 FORMAT(20A4)
  300 FORMAT(5(F5.1,F9.3))
      CALL PLOTS(0,0,0)
       XMIN=9.
       XMAX=XMIN+7.25
       YMIN=0.
       YMAX=YMIN+10.
      CALL WINDOW(XMIN-.5,XMAX,YMIN-.5,YMAX)
      CALL PLOTS(0,0,0)
      CALL GRID(XMIN,0.,70.,1.,-60.,.1666667,4369)
      CALL GRID(XMIN,0.,7,1.,15,.6666667,13107)
C   DRAW X AXIS
      CALL HLINE(XMIN,XMIN+7,0.,65535)
      XCX=XMIN+3.5
      YCX=YMIN-.34
      READ(5,100) H
      CALL CCFONT(XCX,YCX,.15,H,0.,-9,8,0.,1.,.01)
      DO 13 I=1,8
      FPNX=XMIN+(I-1)
      XCNTRX=XMIN+(I-1)
      YCNTRX=YMIN-.15
      CALL VLINE(0.,-.065,XCNTRX,65535)
   13 CALL NCFONT(XCNTRX,YCNTRX,.075,FPNX,0.,1,8,10.,1.,.01)
C  DRAW Y AXIS
      CALL VLINE(0.,10.,XMIN,65535)
      XCY=XMIN-.34
      YCY=YMIN+5.
      READ(5,100) H
      CALL CCFONT(XCY,YCY,.15,H,270.,-9,8,0.,1.,.01)
      XEND=XMIN-.065
      DO 12 I=1,5
      YCNTRY=I*1.6666667
      XCNTRY=XMIN-.15
      FPNY=500.*I
      CALL HLINE(XMIN,XEND,YCNTRY,65535)
      CALL HLINE(XMIN,XMIN+7.,YCNTRY,13107)
   12 CALL NCFONT(XCNTRY,YCNTRY,.075,FPNY,270.,-1,8,10.,1.,.01)
C
C    PLOT COMPARITIVE PATTERNS
C
      CALL NEWPEN(3)
C  5 X 5 X 5
      IN=((XMIN-3.9)/.1)+1
      CALL PLOT(KA1(IN),INT1(IN)/300,3)
      DO 20 I=1,71
      II=I+((XMIN-3.9)/.1)



   20 CALL PLOT(KA1(II),INT1(II)/300,2)
C
      CALL NEWPEN(2)
C  1 X 4 X 18
      CALL PLOT(KA2(IN),INT2(IN)/300,3)
      CALL DSHLNO(.01,.05,KA2(IN),INT2(IN)/300)
      CALL DSHLN1(KA2(IN),INT2(IN)/300)
      DO 21 I=1,71
      II=I+((XMIN-3.9)/.1)
   21 CALL DSHLN(KA2(II),INT2(II)/300)
C   2 X 2 X 20
      CALL PLOT(KA3(IN),INT3(IN)/300,3)
      CALL DSHLNO(.03,.04,KA3(IN),INT3(IN)/300)
      CALL DSHLN1(KA3(IN),INT3(IN)/300)
      DO 22 I=1,71
      II=I+((XMIN-3.9)/.1)
   22 CALL DSHLN(KA3(II),INT3(II)/300)
      CALL NEWPEN(1)
```

```
C  1 X 8 X 8
      CALL PLOT(KA4(IN),INT4(IN)/300.,3)
      DO 23 I=1,71
      II=I+((XMIN-3.9)/.1)
   23 CALL PLOT(KA4(II),INT4(II)/300.,2)
C
C  5 X 5 X 5
      CALL NEWPEN(3)
      READ(5,100) H
      CALL PLOT(XMIN+4.,7.883,3)
      CALL PLOT(XMIN+4.9,7.883,2)
      CALL CLFONT(XMIN+5.,7.833,.1,H,0.,10,8,0.,1.,.01)
      CALL NEWPEN(2)
C  1 X 4 X 18
      READ(5,100) H
      CALL PLOT(XMIN+4.,7.733,3)
      CALL DSHLN0(.01,.05,XMIN+4.,7.733)
      CALL DSHLN1(XMIN+4.,7.733)
      CALL DSHLN(XMIN+4.9,7.733)
      CALL CLFONT(XMIN+5.,7.683,.1,H,0.,10,8,0.,1.,.01)
C  2 X 2 X 20
      READ(5,100) H
      CALL PLOT(XMIN+4.,7.583,3)
      CALL DSHLN0(.03,.04,XMIN+4.,7.583)
      CALL DSHLN1(XMIN+4.,7.583)
      CALL DSHLN(XMIN+4.9,7.583)
      CALL CLFONT(XMIN+5.,7.533,.1,H,0.,10,8,0.,1.,.01)
      CALL NEWPEN(1)
C  1 X 8 X 8
      READ(5,100) H
      CALL PLOT(XMIN+4.,7.433,3)
      CALL PLOT(XMIN+4.9,7.433,2)
      CALL CLFONT(XMIN+5.,7.383,.1,H,0.,10,8,0.,1.,.01)
C
      CALL PLOT(0.,0.,999)
      STOP
      END
/*
//GO.DATA   DD *
          REMOVE THIS CARD AND PUT CRYSTAL DATA CARDS HERE
KA VALUES
INTENSITY
5 X 5 X 5
1 X 4 X 18


2 X 2 X 20
1 X 8 X 8
/*
//
```

APPENDIX B

Shown here is the printout for a 5x5x5 FCC program. Included are listings of the atomic coordinates, the different interatomic distances and their respective frequencies, KA values and intensities, peak values and the intensity maximum for the intensity distribution pattern. Peak values of the other crystallites are provided for comparison.

ATOMIC COORDINATES IN ANGSTROMS

ATOM	X-AXIS	Y-AXIS	Z-AXIS	ATOM	X-AXIS	Y-AXIS	Z-AXIS	ATOM	X-AXIS	Y-AXIS	Z-AX
1	0.0	0.0	0.0	2	0.0	0.0	1.00	3	0.0	0.0	2.00
4	0.0	0.0	3.00	5	0.0	0.0	4.00	6	0.0	0.0	5.00
7	0.0	1.00	0.0	8	0.0	1.00	1.00	9	0.0	1.00	2.00
10	0.0	1.00	3.00	11	0.0	1.00	4.00	12	0.0	1.00	5.00
13	0.0	2.00	0.0	14	0.0	2.00	1.00	15	0.0	2.00	2.00
16	0.0	2.00	3.00	17	0.0	2.00	4.00	18	0.0	2.00	5.00
19	0.0	3.00	0.0	20	0.0	3.00	1.00	21	0.0	3.00	2.00
22	0.0	3.00	3.00	23	0.0	3.00	4.00	24	0.0	3.00	5.00
25	0.0	4.00	0.0	26	0.0	4.00	1.00	27	0.0	4.00	2.00
28	0.0	4.00	3.00	29	0.0	4.00	4.00	30	0.0	4.00	5.00
31	0.0	5.00	0.0	32	0.0	5.00	1.00	33	0.0	5.00	2.00
34	0.0	5.00	3.00	35	0.0	5.00	4.00	36	0.0	5.00	5.00
37	1.00	0.0	0.0	38	1.00	0.0	1.00	39	1.00	0.0	2.00
40	1.00	0.0	3.00	41	1.00	0.0	4.00	42	1.00	0.0	5.00
43	1.00	1.00	0.0	44	1.00	1.00	1.00	45	1.00	1.00	2.00
46	1.00	1.00	3.00	47	1.00	1.00	4.00	48	1.00	1.00	5.00
49	1.00	2.00	0.0	50	1.00	2.00	1.00	51	1.00	2.00	2.00
52	1.00	2.00	3.00	53	1.00	2.00	4.00	54	1.00	2.00	5.00
55	1.00	3.00	0.0	56	1.00	3.00	1.00	57	1.00	3.00	2.00
58	1.00	3.00	3.00	59	1.00	3.00	4.00	60	1.00	3.00	5.00
61	1.00	4.00	0.0	62	1.00	4.00	1.00	63	1.00	4.00	2.00
64	1.00	4.00	3.00	65	1.00	4.00	4.00	66	1.00	4.00	5.00
67	1.00	5.00	0.0	68	1.00	5.00	1.00	69	1.00	5.00	2.00
70	1.00	5.00	3.00	71	1.00	5.00	4.00	72	1.00	5.00	5.00
73	2.00	0.0	0.0	74	2.00	0.0	1.00	75	2.00	0.0	2.00
76	2.00	0.0	3.00	77	2.00	0.0	4.00	78	2.00	0.0	5.00
79	2.00	1.00	0.0	80	2.00	1.00	1.00	81	2.00	1.00	2.00
82	2.00	1.00	3.00	83	2.00	1.00	4.00	84	2.00	1.00	5.00
85	2.00	2.00	0.0	86	2.00	2.00	1.00	87	2.00	2.00	2.00
88	2.00	2.00	3.00	89	2.00	2.00	4.00	90	2.00	2.00	5.00
91	2.00	3.00	0.0	92	2.00	3.00	1.00	93	2.00	3.00	2.00
94	2.00	3.00	3.00	95	2.00	3.00	4.00	96	2.00	3.00	5.00
97	2.00	4.00	0.0	98	2.00	4.00	1.00	99	2.00	4.00	2.00
100	2.00	4.00	3.00	101	2.00	4.00	4.00	102	2.00	4.00	5.00
103	2.00	5.00	0.0	104	2.00	5.00	1.00	105	2.00	5.00	2.00
106	2.00	5.00	3.00	107	2.00	5.00	4.00	108	2.00	5.00	5.00
109	3.00	0.0	0.0	110	3.00	0.0	1.00	111	3.00	0.0	2.00
112	3.00	0.0	3.00	113	3.00	0.0	4.00	114	3.00	0.0	5.00
115	3.00	1.00	0.0	116	3.00	1.00	1.00	117	3.00	1.00	2.00
118	3.00	1.00	3.00	119	3.00	1.00	4.00	120	3.00	1.00	5.00
121	3.00	2.00	0.0	122	3.00	2.00	1.00	123	3.00	2.00	2.00
124	3.00	2.00	3.00	125	3.00	2.00	4.00	126	3.00	2.00	5.00
127	3.00	3.00	0.0	128	3.00	3.00	1.00	129	3.00	3.00	2.00
130	3.00	3.00	3.00	131	3.00	3.00	4.00	132	3.00	3.00	5.00
133	3.00	4.00	0.0	134	3.00	4.00	1.00	135	3.00	4.00	2.00
136	3.00	4.00	3.00	137	3.00	4.00	4.00	138	3.00	4.00	5.00
139	3.00	5.00	0.0	140	3.00	5.00	1.00	141	3.00	5.00	2.00
142	3.00	5.00	3.00	143	3.00	5.00	4.00	144	3.00	5.00	5.00
145	4.00	0.0	0.0	146	4.00	0.0	1.00	147	4.00	0.0	2.00
148	4.00	0.0	3.00	149	4.00	0.0	4.00	150	4.00	0.0	5.00
151	4.00	1.00	0.0	152	4.00	1.00	1.00	153	4.00	1.00	2.00
154	4.00	1.00	3.00	155	4.00	1.00	4.00	156	4.00	1.00	5.00
157	4.00	2.00	0.0	158	4.00	2.00	1.00	159	4.00	2.00	2.00
160	4.00	2.00	3.00	161	4.00	2.00	4.00	162	4.00	2.00	5.00
163	4.00	3.00	0.0	164	4.00	3.00	1.00	165	4.00	3.00	2.00
166	4.00	3.00	3.00	167	4.00	3.00	4.00	168	4.00	3.00	5.00
169	4.00	4.00	0.0	170	4.00	4.00	1.00	171	4.00	4.00	2.00
172	4.00	4.00	3.00	173	4.00	4.00	4.00	174	4.00	4.00	5.00
175	4.00	5.00	0.0	176	4.00	5.00	1.00	177	4.00	5.00	2.00
178	4.00	5.00	3.00	179	4.00	5.00	4.00	180	4.00	5.00	5.00
181	5.00	0.0	0.0	182	5.00	0.0	1.00	183	5.00	0.0	2.00
184	5.00	0.0	3.00	185	5.00	0.0	4.00	186	5.00	0.0	5.00
187	5.00	1.00	0.0	188	5.00	1.00	1.00	189	5.00	1.00	2.00
190	5.00	1.00	3.00	191	5.00	1.00	4.00	192	5.00	1.00	5.00
193	5.00	2.00	0.0	194	5.00	2.00	1.00	195	5.00	2.00	2.00
196	5.00	2.00	3.00	197	5.00	2.00	4.00	198	5.00	2.00	5.00
199	5.00	3.00	0.0	200	5.00	3.00	1.00	201	5.00	3.00	2.00
202	5.00	3.00	3.00	203	5.00	3.00	4.00	204	5.00	3.00	5.00
205	5.00	4.00	0.0	206	5.00	4.00	1.00	207	5.00	4.00	2.00
208	5.00	4.00	3.00	209	5.00	4.00	4.00	210	5.00	4.00	5.00
211	5.00	5.00	0.0	212	5.00	5.00	1.00	213	5.00	5.00	2.00
214	5.00	5.00	3.00	215	5.00	5.00	4.00	216	5.00	5.00	5.00
217	0.0	0.50	0.50	218	0.0	0.50	1.50	219	0.0	0.50	2.50
220	0.0	0.50	3.50	221	0.0	0.50	4.50	222	0.0	1.50	0.50
223	0.0	1.50	1.50	224	0.0	1.50	2.50	225	0.0	1.50	3.50
226	0.0	1.50	4.50	227	0.0	2.50	0.50	228	0.0	2.50	1.50
229	0.0	2.50	2.50	230	0.0	2.50	3.50	231	0.0	2.50	4.50
232	0.0	3.50	0.50	233	0.0	3.50	1.50	234	0.0	3.50	2.50
235	0.0	3.50	3.50	236	0.0	3.50	4.50	237	0.0	4.50	0.50
238	0.0	4.50	1.50	239	0.0	4.50	2.50	240	0.0	4.50	3.50
241	0.0	4.50	4.50	242	1.00	0.50	0.50	243	1.00	0.50	1.50
244	1.00	0.50	2.50	245	1.00	0.50	3.50	246	1.00	0.50	4.50
247	1.00	1.50	0.50	248	1.00	1.50	1.50	249	1.00	1.50	2.50
250	1.00	1.50	3.50	251	1.00	1.50	4.50	252	1.00	2.50	0.50
253	1.00	2.50	1.50	254	1.00	2.50	2.50	255	1.00	2.50	3.50
256	1.00	2.50	4.50	257	1.00	3.50	0.50	258	1.00	3.50	1.50
259	1.00	3.50	2.50	260	1.00	3.50	3.50	261	1.00	3.50	4.50
262	1.00	4.50	0.50	263	1.00	4.50	1.50	264	1.00	4.50	2.50
265	1.00	4.50	3.50	266	1.00	4.50	4.50	267	2.00	0.50	0.50
268	2.00	0.50	1.50	269	2.00	0.50	2.50	270	2.00	0.50	3.50
271	2.00	0.50	4.50	272	2.00	1.50	0.50	273	2.00	1.50	1.50
274	2.00	1.50	2.50	275	2.00	1.50	3.50	276	2.00	1.50	4.50
277	2.00	2.50	0.50	278	2.00	2.50	1.50	279	2.00	2.50	2.50
280	2.00	2.50	3.50	281	2.00	2.50	4.50	282	2.00	3.50	0.50
283	2.00	3.50	1.50	284	2.00	3.50	2.50	285	2.00	3.50	3.50
286	2.00	3.50	4.50	287	2.00	4.50	0.50	288	2.00	4.50	1.50
289	2.00	4.50	2.50	290	2.00	4.50	3.50	291	2.00	4.50	4.50
292	3.00	0.50	0.50	293	3.00	0.50	1.50	294	3.00	0.50	2.50
295	3.00	0.50	3.50	296	3.00	0.50	4.50	297	3.00	1.50	0.50
298	3.00	1.50	1.50	299	3.00	1.50	2.50	300	3.00	1.50	3.50

301	3.00	1.50	4.50	302	3.00	2.50	0.50	303	3.00	2.50	1.50
304	3.00	2.50	2.50	305	3.00	2.50	3.50	306	3.00	2.50	4.50
307	3.00	3.50	0.50	308	3.00	3.50	1.50	309	3.00	3.50	2.50
310	3.00	3.50	3.50	311	3.00	3.50	4.50	312	3.00	4.50	0.50
313	3.00	4.50	1.50	314	3.00	4.50	2.50	315	3.00	4.50	3.50
316	3.00	4.50	4.50	317	4.00	0.50	0.50	318	4.00	0.50	1.50
319	4.00	0.50	2.50	320	4.00	0.50	3.50	321	4.00	0.50	4.50
322	4.00	1.50	0.50	323	4.00	1.50	1.50	324	4.00	1.50	2.50
325	4.00	1.50	3.50	326	4.00	1.50	4.50	327	4.00	1.50	3.50
328	4.00	2.50	1.50	329	4.00	2.50	2.50	330	4.00	2.50	4.50
331	4.00	2.50	4.50	332	4.00	3.50	0.50	333	4.00	3.50	1.50
334	4.00	3.50	2.50	335	4.00	3.50	3.50	336	4.00	3.50	2.50
337	4.00	4.50	0.50	338	4.00	4.50	1.50	339	4.00	4.50	3.50
340	4.00	4.50	3.50	341	4.00	4.50	4.50	342	5.00	0.50	0.50
343	5.00	0.50	1.50	344	5.00	0.50	2.50	345	5.00	0.50	3.50
346	5.00	0.50	4.50	347	5.00	1.50	0.50	348	5.00	1.50	1.50
349	5.00	1.50	2.50	350	5.00	1.50	3.50	351	5.00	1.50	4.50
352	5.00	2.50	0.50	353	5.00	2.50	1.50	354	5.00	2.50	2.50
355	5.00	2.50	3.50	356	5.00	2.50	4.50	357	5.00	3.50	0.50
358	5.00	3.50	1.50	359	5.00	3.50	2.50	360	5.00	3.50	3.50
361	5.00	3.50	4.50	362	5.00	4.50	0.50	363	5.00	4.50	1.50
364	5.00	4.50	2.50	365	5.00	4.50	3.50	366	5.00	4.50	4.50
367	0.50	0.0	0.50	368	0.50	0.0	1.50	369	0.50	0.0	2.50
370	0.50	0.0	3.50	371	0.50	0.0	4.50	372	0.50	1.00	0.50
373	0.50	1.00	1.50	374	0.50	1.00	2.50	375	0.50	1.00	3.50
376	0.50	1.00	4.50	377	0.50	2.00	0.50	378	0.50	2.00	1.50
379	0.50	2.00	2.50	380	0.50	2.00	3.50	381	0.50	2.00	4.50
382	0.50	3.00	0.50	383	0.50	3.00	1.50	384	0.50	3.00	2.50
385	0.50	3.00	3.50	386	0.50	3.00	4.50	387	0.50	4.00	0.50
388	0.50	4.00	1.50	389	0.50	4.00	2.50	390	0.50	4.00	3.50
391	0.50	4.00	4.50	392	0.50	5.00	0.50	393	0.50	5.00	1.50
394	0.50	5.00	2.50	395	0.50	5.00	3.50	396	0.50	5.00	4.50
397	1.50	0.0	0.50	398	1.50	0.0	1.50	399	1.50	0.0	2.50
400	1.50	0.0	3.50	401	1.50	0.0	4.50	402	1.50	1.00	0.50
403	1.50	1.00	1.50	404	1.50	1.00	2.50	405	1.50	1.00	3.50
406	1.50	1.00	4.50	407	1.50	2.00	0.50	408	1.50	2.00	1.50
409	1.50	2.00	2.50	410	1.50	2.00	3.50	411	1.50	2.00	4.50
412	1.50	3.00	0.50	413	1.50	3.00	1.50	414	1.50	3.00	2.50
415	1.50	3.00	3.50	416	1.50	3.00	4.50	417	1.50	4.00	0.50
418	1.50	4.00	1.50	419	1.50	4.00	2.50	420	1.50	4.00	3.50
421	1.50	4.00	4.50	422	1.50	5.00	0.50	423	1.50	5.00	1.50
424	1.50	5.00	2.50	425	1.50	5.00	3.50	426	1.50	5.00	4.50
427	2.50	0.0	0.50	428	2.50	0.0	1.50	429	2.50	0.0	2.50
430	2.50	0.0	3.50	431	2.50	0.0	4.50	432	2.50	1.00	0.50
433	2.50	1.00	1.50	434	2.50	1.00	2.50	435	2.50	1.00	3.50
436	2.50	1.00	4.50	437	2.50	2.00	0.50	438	2.50	2.00	1.50
439	2.50	2.00	2.50	440	2.50	2.00	3.50	441	2.50	2.00	4.50
442	2.50	3.00	0.50	443	2.50	3.00	1.50	444	2.50	3.00	2.50
445	2.50	3.00	3.50	446	2.50	3.00	4.50	447	2.50	4.00	0.50
448	2.50	4.00	1.50	449	2.50	4.00	2.50	450	2.50	4.00	3.50
451	2.50	4.00	4.50	452	2.50	5.00	0.50	453	2.50	5.00	1.50
454	2.50	5.00	2.50	455	2.50	5.00	3.50	456	2.50	5.00	4.50
457	3.50	0.0	0.50	458	3.50	0.0	1.50	459	3.50	0.0	2.50
460	3.50	0.0	3.50	461	3.50	0.0	4.50	462	3.50	1.00	0.50
463	3.50	1.00	1.50	464	3.50	1.00	2.50	465	3.50	1.00	3.50
466	3.50	1.00	4.50	467	3.50	2.00	0.50	468	3.50	2.00	1.50
469	3.50	2.00	2.50	470	3.50	2.00	3.50	471	3.50	2.00	4.50
472	3.50	3.00	0.50	473	3.50	3.00	1.50	474	3.50	3.00	2.50
475	3.50	3.00	3.50	476	3.50	3.00	4.50	477	3.50	4.00	0.50
478	3.50	4.00	1.50	479	3.50	4.00	2.50	480	3.50	4.00	3.50
481	3.50	4.00	4.50	482	3.50	5.00	0.50	483	3.50	5.00	1.50
484	3.50	5.00	2.50	485	3.50	5.00	3.50	486	3.50	5.00	4.50
487	4.50	0.0	0.50	488	4.50	0.0	1.50	489	4.50	0.0	2.50
490	4.50	0.0	3.50	491	4.50	0.0	4.50	492	4.50	1.00	0.50
493	4.50	1.00	1.50	494	4.50	1.00	2.50	495	4.50	1.00	3.50
496	4.50	1.00	4.50	497	4.50	2.00	0.50	498	4.50	2.00	1.50
499	4.50	2.00	2.50	500	4.50	2.00	3.50	501	4.50	2.00	4.50
502	4.50	3.00	0.50	503	4.50	3.00	1.50	504	4.50	3.00	2.50
505	4.50	3.00	3.50	506	4.50	3.00	4.50	507	4.50	4.00	0.50
508	4.50	4.00	1.50	509	4.50	4.00	2.50	510	4.50	4.00	3.50
511	4.50	4.00	4.50	512	4.50	5.00	0.50	513	4.50	5.00	1.50
514	4.50	5.00	2.50	515	4.50	5.00	3.50	516	4.50	5.00	4.50
517	0.50	0.50	0.0	518	0.50	0.50	1.00	519	0.50	0.50	2.00
520	0.50	0.50	3.00	521	0.50	0.50	4.00	522	0.50	0.50	5.00
523	0.50	1.50	0.0	524	0.50	1.50	1.00	525	0.50	1.50	2.00
526	0.50	1.50	3.00	527	0.50	1.50	4.00	528	0.50	1.50	5.00
529	0.50	2.50	0.0	530	0.50	2.50	1.00	531	0.50	2.50	2.00
532	0.50	2.50	3.00	533	0.50	2.50	4.00	534	0.50	2.50	5.00
535	0.50	3.50	0.0	536	0.50	3.50	1.00	537	0.50	3.50	2.00
538	0.50	3.50	3.00	539	0.50	3.50	4.00	540	0.50	3.50	5.00
541	0.50	4.50	0.0	542	0.50	4.50	1.00	543	0.50	4.50	2.00
544	0.50	4.50	3.00	545	0.50	4.50	4.00	546	0.50	4.50	5.00
547	1.50	0.50	0.0	548	1.50	0.50	1.00	549	1.50	0.50	2.00
550	1.50	0.50	3.00	551	1.50	0.50	4.00	552	1.50	0.50	5.00
553	1.50	1.50	0.0	554	1.50	1.50	1.00	555	1.50	1.50	2.00
556	1.50	1.50	3.00	557	1.50	1.50	4.00	558	1.50	1.50	5.00
559	1.50	2.50	0.0	560	1.50	2.50	1.00	561	1.50	2.50	2.00
562	1.50	2.50	3.00	563	1.50	2.50	4.00	564	1.50	2.50	5.00
565	1.50	3.50	0.0	566	1.50	3.50	1.00	567	1.50	3.50	2.00
568	1.50	3.50	3.00	569	1.50	3.50	4.00	570	1.50	3.50	5.00
571	1.50	4.50	0.0	572	1.50	4.50	1.00	573	1.50	4.50	2.00
574	1.50	4.50	3.00	575	1.50	4.50	4.00	576	1.50	4.50	5.00
577	2.50	0.50	0.0	578	2.50	0.50	1.00	579	2.50	0.50	2.00
580	2.50	0.50	3.00	581	2.50	0.50	4.00	582	2.50	0.50	5.00
583	2.50	1.50	0.0	584	2.50	1.50	1.00	585	2.50	1.50	2.00
586	2.50	1.50	3.00	587	2.50	1.50	4.00	588	2.50	1.50	5.00
589	2.50	2.50	0.0	590	2.50	2.50	1.00	591	2.50	2.50	2.00
592	2.50	2.50	3.00	593	2.50	2.50	4.00	594	2.50	2.50	5.00
595	2.50	3.50	0.0	596	2.50	3.50	1.00	597	2.50	3.50	2.00
598	2.50	3.50	3.00	599	2.50	3.50	4.00	600	2.50	3.50	5.00
601	2.50	4.50	0.0	602	2.50	4.50	1.00	603	2.50	4.50	2.00
604	2.50	4.50	3.00	605	2.50	4.50	4.00	606	2.50	4.50	5.00
607	3.50	0.50	0.0	608	3.50	0.50	1.00	609	3.50	0.50	2.00
610	3.50	0.50	3.00	611	3.50	0.50	4.00	612	3.50	0.50	5.00
613	3.50	1.50	0.0	614	3.50	1.50	1.00	615	3.50	1.50	2.00
616	3.50	1.50	3.00	617	3.50	1.50	4.00	618	3.50	1.50	5.00
619	3.50	2.50	0.0	620	3.50	2.50	1.00	621	3.50	2.50	2.00
622	3.50	2.50	3.00	623	3.50	2.50	4.00	624	3.50	2.50	5.00
625	3.50	3.50	0.0	626	3.50	3.50	1.00	627	3.50	3.50	2.00
628	3.50	3.50	3.00	629	3.50	3.50	4.00	630	3.50	3.50	5.00
631	3.50	4.50	0.0	632	3.50	4.50	1.00	633	3.50	4.50	2.00
634	3.50	4.50	3.00	635	3.50	4.50	4.00	636	3.50	4.50	5.00
637	4.50	0.50	0.0	638	4.50	0.50	1.00	639	4.50	0.50	2.00
640	4.50	0.50	3.00	641	4.50	0.50	4.00	642	4.50	0.50	5.00
643	4.50	1.50	0.0	644	4.50	1.50	1.00	645	4.50	1.50	2.00
646	4.50	1.50	3.00	647	4.50	1.50	4.00	648	4.50	1.50	5.00
649	4.50	2.50	0.0	650	4.50	2.50	1.00	651	4.50	2.50	2.00
652	4.50	2.50	3.00	653	4.50	2.50	4.00	654	4.50	2.50	5.00
655	4.50	3.50	0.0	656	4.50	3.50	1.00	657	4.50	3.50	2.00
658	4.50	3.50	3.00	659	4.50	3.50	4.00	660	4.50	3.50	5.00
661	4.50	4.50	0.0	662	4.50	4.50	1.00	663	4.50	4.50	2.00
664	4.50	4.50	3.00	665	4.50	4.50	4.00	666	4.50	4.50	5.00

	INTERATOMIC DISTANCE	FREQUENCY
1	0.0	666.0
2	1.000	3270.0
3	2.000	2544.0
4	3.000	7122.0
5	4.000	1092.0
6	5.000	2358.0
7	1.414	5352.0
8	2.236	8328.0
9	3.162	5952.0
10	4.123	6528.0
11	5.099	4464.0
12	2.828	3240.0
13	3.606	4632.0
14	4.472	2784.0
15	5.385	3480.0
16	4.243	4584.0
17	5.831	1584.0
18	5.657	600.0
19	6.403	960.0
20	7.071	456.0
21	1.732	2920.0
22	2.449	6816.0
23	3.317	4872.0
24	5.196	1488.0
25	3.742	7584.0
26	4.583	4560.0
27	5.477	1536.0
28	4.359	2712.0
29	5.916	1104.0
30	5.745	1584.0
31	6.481	672.0
32	7.141	120.0
33	3.464	1376.0
34	4.899	1776.0
35	4.690	2112.0
36	6.164	864.0
37	6.000	768.0
38	6.708	528.0
39	7.348	96.0
40	6.557	312.0
41	7.681	72.0
42	6.928	112.0
43	7.550	120.0
44	8.124	48.0
45	8.660	8.0
46	0.707	6600.0
47	1.581	10560.0
48	2.550	21360.0
49	3.536	15720.0
50	4.528	4944.0
51	2.121	12624.0
52	2.915	11712.0
53	3.808	4224.0
54	4.743	10464.0
55	4.301	14304.0
56	5.148	4272.0
57	4.950	7872.0
58	5.701	1056.0
59	6.364	840.0
60	1.225	10800.0
61	1.871	17280.0
62	2.739	12960.0
63	3.674	16368.0
64	4.637	11280.0
65	2.345	6912.0
66	3.082	16368.0
67	3.937	14112.0
68	4.848	7296.0
69	4.416	5184.0
70	5.244	7392.0
71	5.050	2928.0
72	5.788	3840.0
73	6.442	1392.0
74	3.240	10080.0
75	4.062	13344.0
76	5.523	4320.0
77	5.339	5520.0
78	6.042	2784.0
79	6.671	336.0
80	3.391	9600.0
81	5.431	3168.0
82	4.183	5760.0
83	5.612	3360.0
84	5.958	1440.0
85	7.036	432.0
86	6.205	1152.0
87	5.874	1728.0
88	6.519	864.0
89	6.964	576.0
90	7.517	144.0
91	6.124	1392.0
92	6.745	480.0
93	6.285	768.0
94	6.892	384.0
95	6.595	576.0
96	7.176	288.0
97	7.583	192.0
98	8.093	48.0

KA	INTENSITY	KA	INTENSITY	KA	INTENSITY	KA	INTENSITY
4.0	178.51	4.1	165.70	4.2	133.52	4.3	91.78
4.4	51.85	4.5	23.33	4.6	11.45	4.7	16.19
4.8	33.02	4.9	54.60	5.0	73.36	5.1	83.52
5.2	82.40	5.3	70.89	5.4	52.66	5.5	32.91
5.6	16.82	5.7	8.15	5.8	8.39	5.9	16.50
6.0	29.47	6.1	43.11	6.2	53.44	6.3	57.69
6.4	54.62	6.5	45.56	6.6	33.20	6.7	21.12
6.8	12.69	6.9	10.06	7.0	13.76	7.1	22.52
7.2	33.72	7.3	44.20	7.4	51.17	7.5	52.96
7.6	49.50	7.7	42.28	7.8	34.03	7.9	28.00
8.0	27.12	8.1	33.47	8.2	47.72	8.3	69.12
8.4	95.73	8.5	124.87	8.6	153.61	8.7	179.63
8.8	201.39	8.9	218.85	9.0	233.34	9.1	247.48
9.2	264.28	9.3	286.30	9.4	314.59	9.5	348.32
9.6	385.35	9.7	424.20	9.8	466.73	9.9	520.76
10.0	600.93	10.1	726.54	10.2	916.51	10.3	1181.28
10.4	1515.35	10.5	1892.53	10.6	2267.03	10.7	2581.09
10.8	2778.04	10.9	2816.89	11.0	2684.32	11.1	2399.51
11.2	2010.52	11.3	1582.76	11.4	1183.78	11.5	868.48
11.6	669.61	11.7	595.18	11.8	632.41	11.9	755.54
12.0	934.02	12.1	1138.36	12.2	1342.81	12.3	1525.11
12.4	1665.86	12.5	1748.34	12.6	1760.22	12.7	1696.22
12.8	1560.42	12.9	1366.77	13.0	1137.17	13.1	897.14
13.2	670.89	13.3	477.02	13.4	325.90	13.5	219.84
13.6	154.55	13.7	121.08	13.8	112.39	13.9	116.89
14.0	127.51	14.1	138.01	14.2	143.83	14.3	142.41
14.4	133.25	14.5	118.00	14.6	99.99	14.7	83.32
14.8	71.76	14.9	67.62	15.0	71.11	15.1	80.24
15.2	91.63	15.3	101.41	15.4	106.57	15.5	105.83
15.6	100.06	15.7	92.00	15.8	85.46	15.9	84.04
16.0	89.94	16.1	103.10	16.2	121.04	16.3	139.64
16.4	154.67	16.5	163.88	16.6	168.88	16.7	176.19
16.8	196.94	16.9	244.87	17.0	332.88	17.1	469.03
17.2	652.90	17.3	873.44	17.4	1109.49	17.5	1332.59
17.6	1512.29	17.7	1622.29	17.8	1645.98	17.9	1580.05
18.0	1435.19	18.1	1233.63	18.2	1004.12	18.3	776.15
18.4	574.33	18.5	414.58	18.6	302.98	18.7	236.68
18.8	206.81	18.9	201.73	19.0	210.04	19.1	222.56
19.2	233.17	19.3	238.86	19.4	239.62	19.5	238.37
19.6	241.15	19.7	257.27	19.8	298.84	19.9	379.28
20.0	510.62	20.1	700.13	20.2	946.62	20.3	1238.24
20.4	1552.41	20.5	1858.02	20.6	2120.86	20.7	2309.82
20.8	2403.46	20.9	2394.68	21.0	2292.02	21.1	2117.41
21.2	1900.89	21.3	1673.56	21.4	1460.87	21.5	1278.37
21.6	1130.26	21.7	1011.51	21.8	911.96	21.9	820.83
22.0	730.58	22.1	638.29	22.2	545.38	22.3	455.72
22.4	373.51	22.5	301.78	22.6	241.97	22.7	194.27
22.8	158.40	22.9	134.00	23.0	120.54	23.1	116.71
23.2	119.91	23.3	126.20	23.4	131.07	23.5	130.55
23.6	122.63	23.7	107.95	23.8	89.89	23.9	73.61
24.0	64.65	24.1	67.49	24.2	84.62	24.3	116.17
24.4	160.18	24.5	213.29	24.6	271.38	24.7	330.13
24.8	385.28	24.9	432.85	25.0	469.16	25.1	491.11
25.2	496.56	25.3	484.70	25.4	456.45	25.5	414.67
25.6	363.90	25.7	300.99	25.8	259.19	25.9	217.31
26.0	188.97	26.1	177.19	26.2	183.48	26.3	208.54
26.4	252.98	26.5	318.00	26.6	405.54	26.7	517.57
26.8	654.90	26.9	815.77	27.0	994.64	27.1	1162.11
27.2	1365.87	27.3	1532.74	27.4	1671.10	27.5	1772.97
27.6	1835.06	27.7	1858.37	27.8	1846.68	27.9	1804.45
28.0	1734.94	28.1	1639.48	28.2	1518.07	28.3	1371.08
28.4	1201.21	28.5	1015.32	28.6	824.39	28.7	642.36
28.8	483.36	28.9	358.47	29.0	273.15	29.1	225.94
29.2	209.22	29.3	211.55	29.4	221.16	29.5	229.37
29.6	232.91	29.7	234.59	29.8	242.19	29.9	265.84
30.0	314.71	30.1	394.05	30.2	503.15	30.3	634.64
30.4	775.46	30.5	908.94	30.6	1017.63	30.7	1086.50
30.8	1105.45	30.9	1071.25	31.0	988.14	31.1	867.22
31.2	724.67	31.3	579.28	31.4	449.53	31.5	361.28
31.6	295.90	31.7	269.53	31.8	333.01	31.9	422.54
32.0	550.15	32.1	704.38	32.2	870.90	32.3	1033.03
32.4	1173.21	32.5	1274.73	32.6	1324.25	32.7	1314.21
32.8	1244.62	32.9	1123.40	33.0	965.31	33.1	789.26
33.2	614.73	33.3	458.53	33.4	332.08	33.5	240.41
33.6	182.37	33.7	152.18	33.8	141.57	33.9	141.83
34.0	145.63	34.1	147.99	34.2	146.76	34.3	142.32
34.4	137.05	34.5	134.45	34.6	138.24	34.7	151.62
34.8	176.67	34.9	213.96	35.0	262.42	35.1	319.26
35.2	380.14	35.3	439.21	35.4	489.81	35.5	525.19
35.6	538.82	35.7	530.91	35.8	499.85	35.9	452.96
36.0	401.50	36.1	360.22	36.2	345.01	36.3	370.01
36.4	444.77	36.5	572.16	36.6	747.59	36.7	959.60
36.8	1191.33	36.9	1423.03	37.0	1634.32	37.1	1806.60
37.2	1925.05	37.3	1979.86	37.4	1967.31	37.5	1890.03
37.6	1756.70	37.7	1580.87	37.8	1379.22	37.9	1169.09
38.0	966.17	38.1	782.50	38.2	625.27	38.3	497.12
38.4	397.13	38.5	322.71	38.6	271.37	38.7	241.86
38.8	234.45	38.9	250.22	39.0	299.63	39.1	351.09
39.2	430.08	39.3	518.97	39.4	607.95	39.5	686.42
39.6	744.75	39.7	775.91	39.8	776.41	39.9	746.87
40.0	691.91	40.1	619.70	40.2	541.07	40.3	468.42
40.4	414.16	40.5	389.04	40.6	400.19	40.7	449.67
40.8	533.51	40.9	642.05	41.0	761.24	41.1	875.03
41.2	960.36	41.3	1029.56	41.4	1052.29	41.5	1035.90
41.6	984.81	41.7	906.85	41.8	811.31	41.9	707.23
42.0	602.26	42.1	502.28	42.2	411.44	42.3	332.70
42.4	268.17	42.5	219.31	42.6	186.98	42.7	171.15
42.8	170.71	42.9	183.31	43.0	205.41	43.1	232.53
43.2	259.72	43.3	282.27	43.4	296.53	43.5	300.79
43.6	295.92	43.7	285.87	43.8	277.40	43.9	279.46
44.0	301.65	44.1	352.47	44.2	437.30	44.3	536.73
44.4	705.48	44.5	872.65	44.6	1042.70	44.7	1197.96
44.8	1321.19	44.9	1398.73	45.0	1422.68	45.1	1392.03
45.2	1312.35	45.3	1194.41	45.4	1051.80	45.5	898.52
45.6	747.25	45.7	608.30	45.8	489.73	45.9	397.91
46.0	338.08	46.1	314.56	46.2	330.06	46.3	384.58
46.4	473.94	46.5	589.08	46.6	716.25	46.7	838.69
46.8	939.32	46.9	1004.23	47.0	1025.92	47.1	1005.37
47.2	952.57	47.3	884.90	47.4	823.72	47.5	709.70
47.6	798.06	47.7	854.66	47.8	954.12	47.9	1080.34
48.0	1209.86	48.1	1316.53	48.2	1377.40	48.3	1377.47
48.4	1312.69	48.5	1190.26	48.6	1026.57	48.7	842.93
48.8	661.11	48.9	499.09	49.0	368.39	49.1	273.52
49.2	212.82	49.3	180.59	49.4	169.41	49.5	172.06
49.6	182.63	49.7	196.89	49.8	211.99	49.9	225.99
50.0	237.54						

INTENSITY MAXIMUM OF 2816.89 AT A KA VALUE OF 10.9

THERE IS A PEAK OF INTENSITY OF	83.52	AT A KA VALUE OF	5.1	1
THERE IS A PEAK OF INTENSITY OF	57.60	AT A KA VALUE OF	6.3	2
THERE IS A PEAK OF INTENSITY OF	52.96	AT A KA VALUE OF	7.5	3
THERE IS A PEAK OF INTENSITY OF	2816.89	AT A KA VALUE OF	10.9	4
THERE IS A PEAK OF INTENSITY OF	1760.22	AT A KA VALUE OF	12.6	5
THERE IS A PEAK OF INTENSITY OF	143.83	AT A KA VALUE OF	14.2	6
THERE IS A PEAK OF INTENSITY OF	106.57	AT A KA VALUE OF	15.4	7
THERE IS A PEAK OF INTENSITY OF	1645.98	AT A KA VALUE OF	17.8	8
THERE IS A PEAK OF INTENSITY OF	239.62	AT A KA VALUE OF	19.4	9
THERE IS A PEAK OF INTENSITY OF	2403.46	AT A KA VALUE OF	20.8	10
THERE IS A PEAK OF INTENSITY OF	131.07	AT A KA VALUE OF	23.4	11
THERE IS A PEAK OF INTENSITY OF	496.56	AT A KA VALUE OF	25.2	12
THERE IS A PEAK OF INTENSITY OF	1858.37	AT A KA VALUE OF	27.7	13
THERE IS A PEAK OF INTENSITY OF	1105.45	AT A KA VALUE OF	30.8	14
THERE IS A PEAK OF INTENSITY OF	1324.25	AT A KA VALUE OF	32.6	15
THERE IS A PEAK OF INTENSITY OF	147.99	AT A KA VALUE OF	34.1	16
THERE IS A PEAK OF INTENSITY OF	539.82	AT A KA VALUE OF	35.6	17
THERE IS A PEAK OF INTENSITY OF	1979.86	AT A KA VALUE OF	37.3	18
THERE IS A PEAK OF INTENSITY OF	776.41	AT A KA VALUE OF	39.8	19
THERE IS A PEAK OF INTENSITY OF	1052.29	AT A KA VALUE OF	41.4	20
THERE IS A PEAK OF INTENSITY OF	300.79	AT A KA VALUE OF	43.5	21
THERE IS A PEAK OF INTENSITY OF	1422.68	AT A KA VALUE OF	45.0	22
THERE IS A PEAK OF INTENSITY OF	1025.92	AT A KA VALUE OF	47.0	23
THERE IS A PEAK OF INTENSITY OF	1377.47	AT A KA VALUE OF	48.3	24

5 X 5 X 5 FCC

INTENSITY MAXIMUM OF 0.1690197 3E+04 AT A KA VALUE OF 12.6

THERE IS A PEAK OF INTENSITY OF 0.59422E+02AT A KA VALUE OF 5.3	1
THERE IS A PEAK OF INTENSITY OF 0.76049E+02AT A KA VALUE OF 6.3	2
THERE IS A PEAK OF INTENSITY OF 0.55213E+02AT A KA VALUE OF 7.7	3
THERE IS A PEAK OF INTENSITY OF 0.11365E+04AT A KA VALUE OF 10.6	4
THERE IS A PEAK OF INTENSITY OF 0.77345E+03AT A KA VALUE OF 12.1	5
THERE IS A PEAK OF INTENSITY OF 0.16902E+04AT A KA VALUE OF 12.6	6
THERE IS A PEAK OF INTENSITY OF 0.78800E+03AT A KA VALUE OF 17.8	7
THERE IS A PEAK OF INTENSITY OF 0.12608E+04AT A KA VALUE OF 20.8	8
THERE IS A PEAK OF INTENSITY OF 0.51596E+03AT A KA VALUE OF 25.2	9
THERE IS A PEAK OF INTENSITY OF 0.10518E+04AT A KA VALUE OF 28.0	10
THERE IS A PEAK OF INTENSITY OF 0.52418E+03AT A KA VALUE OF 30.8	11
THERE IS A PEAK OF INTENSITY OF 0.75422E+03AT A KA VALUE OF 32.6	12
THERE IS A PEAK OF INTENSITY OF 0.10089E+04AT A KA VALUE OF 37.2	13
THERE IS A PEAK OF INTENSITY OF 0.96447E+03AT A KA VALUE OF 37.6	14
THERE IS A PEAK OF INTENSITY OF 0.58746E+03AT A KA VALUE OF 39.8	15
THERE IS A PEAK OF INTENSITY OF 0.54370E+03AT A KA VALUE OF 41.5	16
THERE IS A PEAK OF INTENSITY OF 0.82704E+03AT A KA VALUE OF 44.9	17
THERE IS A PEAK OF INTENSITY OF 0.76736E+03AT A KA VALUE OF 48.2	18

1 X 4 X 18 FCC

INTENSITY MAXIMUM OF C.17850322E+04 AT A KA VALUE OF 12.6

THERE IS A PEAK OF INTENSITY OF	0.71194E+02AT A KA VALUE OF 6.3	1
THERE IS A PEAK OF INTENSITY OF	0.1327CE+04AT A KA VALUE OF 10.9	2
THERE IS A PEAK OF INTENSITY OF	C.17850E+04AT A KA VALUE OF 12.6	3
THERE IS A PEAK OF INTENSITY OF	0.57071E+03AT A KA VALUE OF 13.1	4
THERE IS A PEAK OF INTENSITY OF	0.12C53E+03AT A KA VALUE OF 15.5	5
THERE IS A PEAK OF INTENSITY OF	0.7C957E+03AT A KA VALUE OF 17.7	6
THERE IS A PEAK OF INTENSITY OF	0.13967E+04AT A KA VALUE OF 20.9	7
THERE IS A PEAK OF INTENSITY OF	0.2133CE+03AT A KA VALUE OF 24.7	8
THERE IS A PEAK OF INTENSITY OF	0.52973E+03AT A KA VALUE OF 25.2	9
THERE IS A PEAK OF INTENSITY OF	0.11C04E+04AT A KA VALUE OF 27.9	10
THERE IS A PEAK OF INTENSITY OF	0.57258E+03AT A KA VALUE OF 30.9	11
THERE IS A PEAK OF INTENSITY OF	0.81231E+03AT A KA VALUE OF 32.6	12
THERE IS A PEAK OF INTENSITY OF	0.1C393E+04AT A KA VALUE OF 37.3	13
THERE IS A PEAK OF INTENSITY OF	0.1C61CE+04AT A KA VALUE OF 37.7	14
THERE IS A PEAK OF INTENSITY OF	0.51912E+03AT A KA VALUE OF 39.8	15
THERE IS A PEAK OF INTENSITY OF	0.59735E+03AT A KA VALUE OF 41.4	16
THERE IS A PEAK OF INTENSITY OF	0.88554E+03AT A KA VALUE OF 44.9	17
THERE IS A PEAK OF INTENSITY OF	0.81526E+03AT A KA VALUE OF 48.1	18

2 X 2 X 20 FCC

INTENSITY MAXIMUM OF 0.12785662E+04 AT A KA VALUE OF 12.6

THERE IS A PEAK OF INTENSITY OF	0.42039E+02 AT A KA VALUE OF 5.0	1
THERE IS A PEAK OF INTENSITY OF	0.58122E+02 AT A KA VALUE OF 5.7	2
THERE IS A PEAK OF INTENSITY OF	0.62187E+02 AT A KA VALUE OF 6.3	3
THERE IS A PEAK OF INTENSITY OF	0.43583E+02 AT A KA VALUE OF 7.0	4
THERE IS A PEAK OF INTENSITY OF	0.99751E+03 AT A KA VALUE OF 10.7	5
THERE IS A PEAK OF INTENSITY OF	0.12786E+04 AT A KA VALUE OF 12.6	6
THERE IS A PEAK OF INTENSITY OF	0.19299E+03 AT A KA VALUE OF 13.7	7
THERE IS A PEAK OF INTENSITY OF	0.81035E+03 AT A KA VALUE OF 17.8	8
THERE IS A PEAK OF INTENSITY OF	0.11440E+04 AT A KA VALUE OF 20.8	9
THERE IS A PEAK OF INTENSITY OF	0.36940E+03 AT A KA VALUE OF 25.2	10
THERE IS A PEAK OF INTENSITY OF	0.96490E+03 AT A KA VALUE OF 28.1	11
THERE IS A PEAK OF INTENSITY OF	0.46033E+03 AT A KA VALUE OF 30.8	12
THERE IS A PEAK OF INTENSITY OF	0.67974E+03 AT A KA VALUE OF 32.6	13
THERE IS A PEAK OF INTENSITY OF	0.36555E+03 AT A KA VALUE OF 35.7	14
THERE IS A PEAK OF INTENSITY OF	0.91901E+03 AT A KA VALUE OF 37.3	15
THERE IS A PEAK OF INTENSITY OF	0.51555E+03 AT A KA VALUE OF 39.8	16
THERE IS A PEAK OF INTENSITY OF	0.48192E+03 AT A KA VALUE OF 41.5	17
THERE IS A PEAK OF INTENSITY OF	0.73882E+03 AT A KA VALUE OF 45.0	18
THERE IS A PEAK OF INTENSITY OF	0.55290E+03 AT A KA VALUE OF 47.2	19
THERE IS A PEAK OF INTENSITY OF	0.69193E+03 AT A KA VALUE OF 48.2	20

1 X 8 X 8 FCC

INTENSITY MAXIMUM OF 0.7C0463206+03 AT A KA VALUE OF 12.7

THERE IS A PEAK OF INTENSITY OF 0.582347+02AT A KA VALUE OF 6.4 1
THERE IS A PEAK OF INTENSITY OF 0.434732+02AT A KA VALUE OF 10.8 2
THERE IS A PEAK OF INTENSITY OF 0.700479+03AT A KA VALUE OF 12.7 3
THERE IS A PEAK OF INTENSITY OF 0.141239+03AT A KA VALUE OF 13.7 4
THERE IS A PEAK OF INTENSITY OF 0.243398+03AT A KA VALUE OF 18.3 5
THERE IS A PEAK OF INTENSITY OF 0.242798+03AT A KA VALUE OF 18.8 6
THERE IS A PEAK OF INTENSITY OF 0.426706+03AT A KA VALUE OF 20.8 7
THERE IS A PEAK OF INTENSITY OF 0.263486+03AT A KA VALUE OF 25.2 8
THERE IS A PEAK OF INTENSITY OF 0.263547+03AT A KA VALUE OF 27.8 9
THERE IS A PEAK OF INTENSITY OF 0.227346+03AT A KA VALUE OF 31.1 10
THERE IS A PEAK OF INTENSITY OF 0.284956+03AT A KA VALUE OF 32.5 11
THERE IS A PEAK OF INTENSITY OF 0.337626+03AT A KA VALUE OF 37.2 12
THERE IS A PEAK OF INTENSITY OF 0.290706+03AT A KA VALUE OF 37.7 13
THERE IS A PEAK OF INTENSITY OF 0.230976+03AT A KA VALUE OF 39.7 14
THERE IS A PEAK OF INTENSITY OF 0.213696+03AT A KA VALUE OF 41.5 15
THERE IS A PEAK OF INTENSITY OF 0.302536+03AT A KA VALUE OF 44.9 16
THERE IS A PEAK OF INTENSITY OF 0.273426+03AT A KA VALUE OF 46.3 17
THERE IS A PEAK OF INTENSITY OF 0.291126+03AT A KA VALUE OF 47.3 18

1 X 1 X 25 FCC

APPENDIX C

This is a derivation of the equation

$$KA = 2\pi(h^2+k^2+l^2)^{\frac{1}{2}}$$

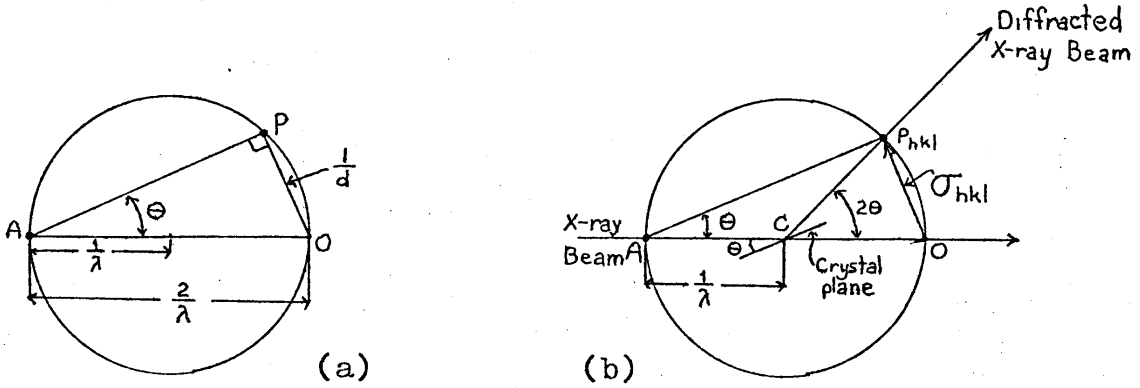
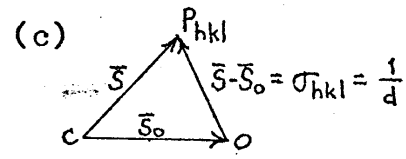


Figure 14.



$$\lambda = 2d\sin\Theta$$

$$\frac{1}{d} = \frac{2\sin\Theta}{\lambda}$$

$$\left|\bar{S}-\bar{S}_o\right| = \frac{2\sin\Theta}{\lambda} = \frac{1}{d}$$

$$K = \frac{4\pi\sin\Theta}{\lambda} = 2\pi\left(\frac{2\sin\Theta}{\lambda}\right) = 2\pi\left(\frac{1}{d}\right) \qquad \text{(A-1)}$$

Combining $\bar{\sigma}_{hkl} = M\frac{1}{d_{hkl}}$ and $\bar{\sigma}_{hkl} = ha^*+kb^*+lc^*$, where M is a scale factor for the reciprocal-lattice treatment of the crystal lattice, and a*, b*, c* represent the reciprocal-lattice axes, will give the following solution.

$$\bar{\sigma}_{hkl} \cdot \bar{\sigma}_{hkl} = (ha^* + kb^* + lc^*)\cdot(ha^* + kb^* + lc^*)$$

Since in the Isometric system $a^*=b^*=c^*$ and all interaxial angles are equal to 90°, carrying out the dot product gives:

$$\sigma_{hkl}^2 = \frac{1}{d_{hkl}^2} = (h^2+k^2+l^2)a^{*2} \quad .$$

In the Isometric system $a^* = \frac{1}{d_{100}} = \frac{1}{a}$, so

$$\frac{1}{d^2} = \frac{h^2+k^2+l^2}{a^2}$$

$$\frac{1}{d} = \frac{(h^2+k^2+l^2)^{\frac{1}{2}}}{a} \qquad \text{(A-2)}$$

Substituting (A-2) into (A-1) results in

$$K = 2\pi \frac{(h^2+k^2+l^2)^{\frac{1}{2}}}{a} \quad , \text{ or for use when } A=a$$

$$KA = 2\pi (h^2+k^2+l^2)^{\frac{1}{2}}$$

APPENDIX D

$h^2+k^2+l^2$	hkl	KA value	p	Possible reflections for lattice type FCC	BCC	PI
1	100	6.28	6			*
2	110	8.88	12		*	*
3	111	10.88	8	*		*
4	200	12.57	6	*	*	*
5	210	14.05	24			*
6	211	15.39	24		*	*
8	220	17.77	12	*	*	*
9	300,221	18.85	30			*
10	310	19.87	24		*	*
11	311	20.84	24	*		*
12	222	21.77	8	*	*	*
13	320	22.65	24			*
14	321	23.51	48		*	*
16	400	25.13	6	*	*	*
17	410,322	25.91	48			*
18	411.330	26.66	36		*	*
19	331	27.39	24	*		*
20	420	28.10	24	*	*	*
21	421	28.79	48			*
22	332	29.47	24		*	*
24	422	30.78	24	*	*	*
25	500,430	31.42	30			*
26	510,431	32.04	72		*	*
27	511,333	32.65	32	*		*
29	520,432	33.84	72			*
30	521	34.41	48		*	*
32	440	35.54	12	*	*	*
33	522,441	36.09	48			*
34	530,433	36.64	48		*	*
35	531	37.17	48	*		*
36	600,442	37.70	30	*	*	*
37	610	38.22	24			*
38	611,532	38.73	72		*	*
40	620	39.74	24	*	*	*
41	621,540,443	40.23	96			*
42	541	40.72	48		*	*
43	533	41.20	24	*		*
44	622	41.68	24	*	*	*

$h^2+k^2+l^2$	hkl	KA value	p	Possible reflections for lattice type FCC	BCC	PI
45	630,542	42.15	72			*
46	631	42.61	48		*	*
48	444	43.53	8	*	*	*
49	700,632	43.98	54			*
50	710,550,543	44.43	84		*	*
51	711,551	44.87	48	*		*
52	640	45.30	24	*	*	*
53	720,641	45.74	72			*
54	721,633,552	46.17	96		*	*
56	642	47.02	48	*	*	*
57	722,544	47.44	48			*
58	730	47.85	24		*	*
59	731,553	48.26	72	*		*

hkl = Miller indices of the reflecting plane of atoms

$KA = 2\pi(h^2+k^2+l^2)^{\frac{1}{2}}$

p = multiplicity factor, i.e. the relative proportion of planes contributing to the same reflection. The value of p depends on the crystal system. The values given here are for the Isometric system obtained from Cullity (p.523). If two or more reflections plot at the same KA value, the relative intensity is the sum of the multiplicities.

APPENDIX E

Summary of computer processing. All runs required just over 200 K of sustem storage.

Lattice type	Crystallite size	Time execution (min.)	CPU (min:sec)	Number of atoms	Number of unique distances
PI	7x7x7	2.83	0:13.96	343	67
BCC	6x6x6	12.56	1:04.93	559	103
FCC	1x1x1	0.20	0:01.20	14	6
FCC	1x8x8	4.54	1:00.80	434	156
FCC	2x2x20	7.94	2:22.41	513	277
FCC	1x4x18	10.42	2:42.13	500	342
FCC	5x5x5	22.53	1:36.58	666	98
FCC	5x5x5*	2.81	1:32.57	666	98

* This run of a 5x5x5 was with the same program as the others but the KA values were calculated in increments of 0.2 rather 0.1 (as the others were) and there were no cards punched.

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